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11-1160

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## Scientific and Technical Information Center

## SEARCH REQUEST FORM

Requester's Full Name: MARK BERCH Examiner #: 59193 Date: 11/27/06  
 Art Unit: 1624 Phone Number: 2-0663 Serial Number: 10044486  
 Location (Bldg/Room#): 5C01 (Mailbox #): 5C18 Results Format Preferred (circle): PAPER DISK  
 \*\*\*\*\*

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: \_\_\_\_\_

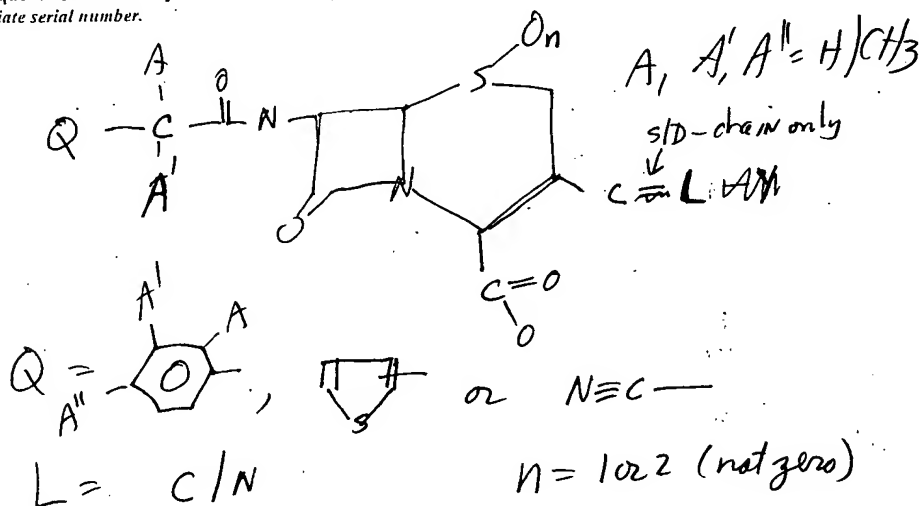
Inventors (please provide full names): \_\_\_\_\_

Earliest Priority Date: \_\_\_\_\_

## Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.



Compound must have linked to it one of those terms: fluorogenic, fluorescent, dye, chromophore

## STAFF USE ONLY

Searcher: \_\_\_\_\_

Searcher Phone #: \_\_\_\_\_

Searcher Location: \_\_\_\_\_

Date Searcher Picked Up: \_\_\_\_\_

Date Completed: 12/11

Searcher Prep & Review Time: \_\_\_\_\_

Online Time: 25

## Type of Search

\_\_\_\_ NA Sequence (#)

\_\_\_\_ AA Sequence (#)

1 Structure (#)

\_\_\_\_ Bibliographic

\_\_\_\_ Litigation

\_\_\_\_ Fulltext

\_\_\_\_ Other

## Vendors and cost where applicable

297.07 STN \_\_\_\_\_ Dialog

\_\_\_\_ Questel/Orbit \_\_\_\_\_ Lexis/Nexis

\_\_\_\_ Westlaw \_\_\_\_\_ WWW/Internet

\_\_\_\_ In-house sequence systems

\_\_\_\_ Commercial \_\_\_\_\_ Oligomer \_\_\_\_\_ Score/Length

\_\_\_\_ Interference \_\_\_\_\_ SPDI \_\_\_\_\_ Encode/Transl

\_\_\_\_ Other (specify)

=> file registry

FILE 'REGISTRY' ENTERED AT 14:49:25 ON 11 DEC 2006  
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STRUCTURE FILE UPDATES: 10 DEC 2006 HIGHEST RN 915124-84-4  
DICTIONARY FILE UPDATES: 10 DEC 2006 HIGHEST RN 915124-84-4

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TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

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=> file caplus

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FILE COVERS 1907 - 11 Dec 2006 VOL 145 ISS 25  
FILE LAST UPDATED: 10 Dec 2006 (20061210/ED)

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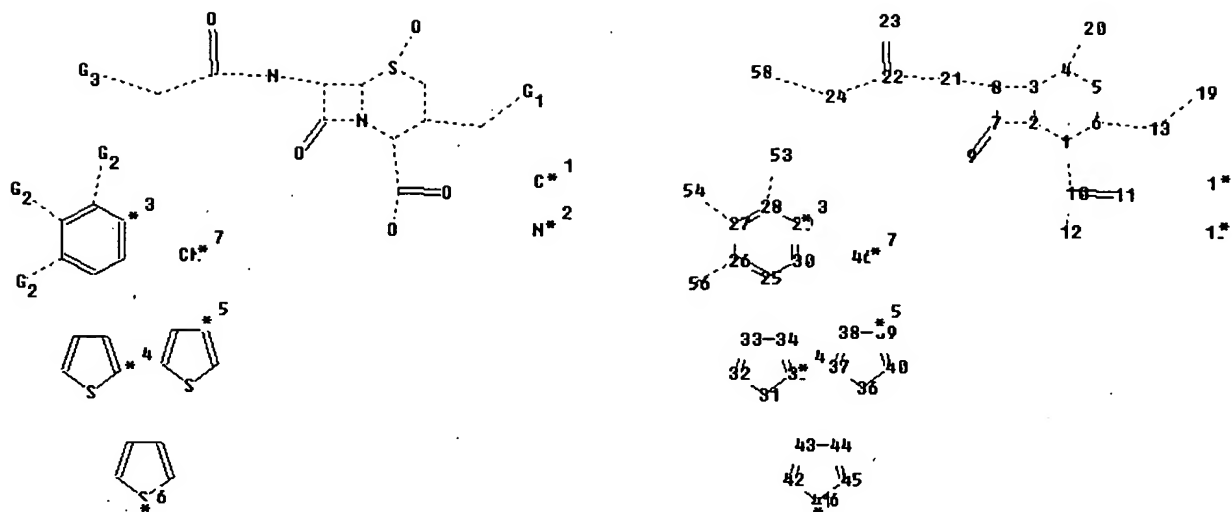
'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> d stat que L10

L1 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation:  
Uploading L1.str



chain nodes :

9 10 11 12 13 19 20 21 22 23 24 46 53 54 56 58

ring nodes :

1 2 3 4 5 6 7 8 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39  
40 41 42 43 44 45

ring/chain nodes :

14 15

chain bonds :

1-10 4-20 6-13 7-9 8-21 10-11 10-12 13-19 21-22 22-23 22-24 24-58 26-56  
27-54 28-53

ring bonds :

1-2 1-6 2-3 2-7 3-4 3-8 4-5 5-6 7-8 25-26 25-30 26-27 27-28 28-29 29-30

31-32 31-35 32-33 33-34 34-35 36-37 36-40 37-38 38-39 39-40 41-42 41-45  
42-43 43-44

44-45

exact/norm bonds :

1-2 1-6 1-10 2-3 2-7 3-4 3-8 4-5 4-20 5-6 6-13 7-8 7-9 8-21 10-11  
10-12 13-19 21-22 22-23 22-24 24-58 26-56 27-54 28-53 31-32 31-35 32-33  
33-34 34-35 36-37  
36-40 37-38 38-39 39-40 41-42 41-45 42-43 43-44 44-45

normalized bonds :

25-26 25-30 26-27 27-28 28-29 29-30

G1: [\*1], [\*2]

G2: H, CH3

G3: [\*3], [\*4], [\*5], [\*6], [\*7]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS

11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 19:CLASS 20:CLASS 21:CLASS  
 22:CLASS 23:CLASS  
 24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom  
 33:Atom 34:Atom  
 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom  
 44:Atom 45:Atom  
 46:CLASS 53:CLASS 54:CLASS 56:CLASS 58:CLASS

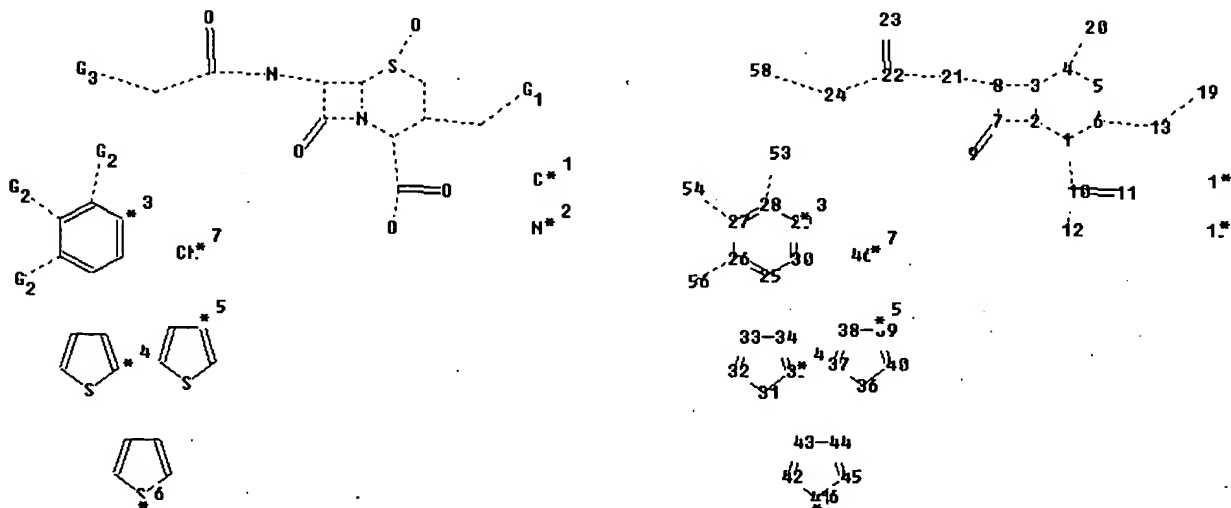
L3 178 SEA FILE=REGISTRY SSS FUL L1  
 L4 82 SEA FILE=CAPLUS ABB=ON PLU=ON L3  
 L5 4869 SEA FILE=CAPLUS ABB=ON PLU=ON ?FLUOROGEN?/BI  
 L6 484544 SEA FILE=CAPLUS ABB=ON PLU=ON ?FLUORESCEN?/BI  
 L7 380423 SEA FILE=CAPLUS ABB=ON PLU=ON DYE?/BI  
 L8 381931 SEA FILE=CAPLUS ABB=ON PLU=ON ?DYE?/BI  
 L9 39403 SEA FILE=CAPLUS ABB=ON PLU=ON ?CHROMOPHOR?/BI  
 L10 7 SEA FILE=CAPLUS ABB=ON PLU=ON L4 AND (L5 OR L6 OR L7 OR L8 OR L9)

=> d stat que L14

L1 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation:  
 Uploading L1.str



chain nodes :

9 10 11 12 13 19 20 21 22 23 24 46 53 54 56 58

ring nodes :

1 2 3 4 5 6 7 8 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39

```

40 41 42 43 44 45
ring/chain nodes :
14 15
chain bonds :
1-10 4-20 6-13 7-9 8-21 10-11 10-12 13-19 21-22 22-23 22-24 24-58 26-56
27-54 28-53
ring bonds :
1-2 1-6 2-3 2-7 3-4 3-8 4-5 5-6 7-8 25-26 25-30 26-27 27-28 28-29 29-
30
31-32 31-35 32-33 33-34 34-35 36-37 36-40 37-38 38-39 39-40 41-42 41-45
42-43 43-44
44-45
exact/norm bonds :
1-2 1-6 1-10 2-3 2-7 3-4 3-8 4-5 4-20 5-6 6-13 7-8 7-9 8-21 10-11
10-12 13-19 21-22 22-23 22-24 24-58 26-56 27-54 28-53 31-32 31-35 32-33
33-34 34-35 36-37
36-40 37-38 38-39 39-40 41-42 41-45 42-43 43-44 44-45
normalized bonds :
25-26 25-30 26-27 27-28 28-29 29-30

```

G1:[\*1],[\*2]

G2:H,CH3

G3:[\*3],[\*4],[\*5],[\*6],[\*7]

Match level :

```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 19:CLASS 20:CLASS 21:CLASS
22:CLASS 23:CLASS
24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom
33:Atom 34:Atom
35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom
44:Atom 45:Atom
46:CLASS 53:CLASS 54:CLASS 56:CLASS 58:CLASS

```

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L3          178 SEA FILE=REGISTRY SSS FUL L1
L4          82 SEA FILE=CAPLUS ABB=ON PLU=ON L3
L13         11130 SEA FILE=CAPLUS ABB=ON PLU=ON ?FLUOROPHOR?/BI
L14         1 SEA FILE=CAPLUS ABB=ON PLU=ON L4 AND L13

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=> file uspatfull

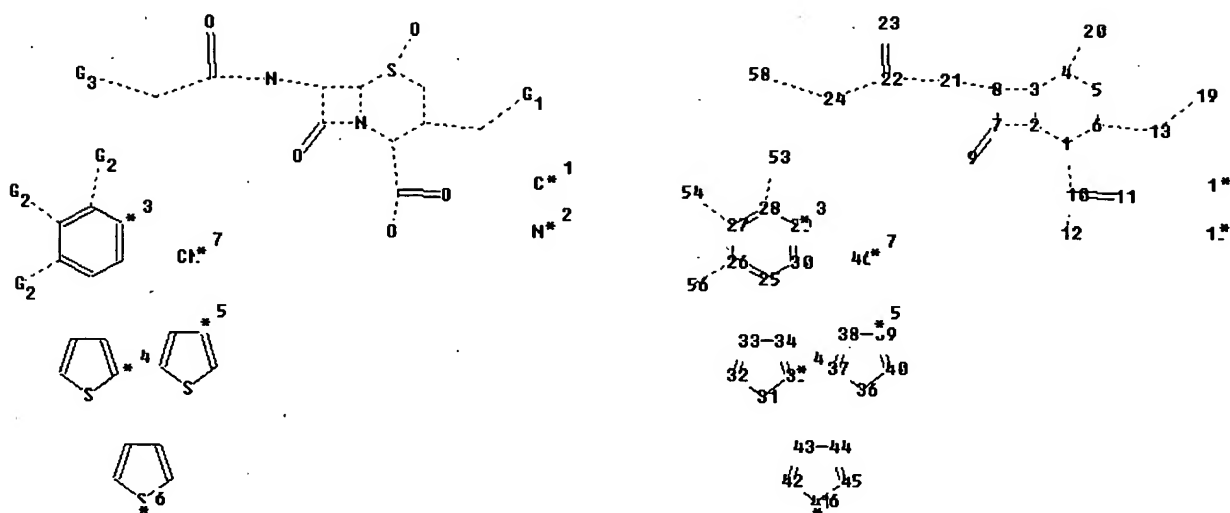
FILE 'USPATFULL' ENTERED AT 14:51:22 ON 11 DEC 2006  
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FILE COVERS 1971 TO PATENT PUBLICATION DATE: 7 Dec 2006 (20061207/PD)  
FILE LAST UPDATED: 7 Dec 2006 (20061207/ED)  
HIGHEST GRANTED PATENT NUMBER: US7146645  
HIGHEST APPLICATION PUBLICATION NUMBER: US2006277640  
CA INDEXING IS CURRENT THROUGH 7 Dec 2006 (20061207/UPCA)  
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 7 Dec 2006 (20061207/PD)  
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2006  
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2006

=> d stat que L23  
L1 STR

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Structure attributes must be viewed using STN Express query preparation:  
Uploading L1.str



chain nodes :

9 10 11 12 13 19 20 21 22 23 24 46 53 54 56 58

ring nodes :

1 2 3 4 5 6 7 8 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39  
40 41 42 43 44 45

ring/chain nodes :

14 15

chain bonds :

1-10 4-20 6-13 7-9 8-21 10-11 10-12 13-19 21-22 22-23 22-24 24-58 26-56  
27-54 28-53

ring bonds :

1-2 1-6 2-3 2-7 3-4 3-8 4-5 5-6 7-8 25-26 25-30 26-27 27-28 28-29 29-30

31-32 31-35 32-33 33-34 34-35 36-37 36-40 37-38 38-39 39-40 41-42 41-45  
42-43 43-44

44-45

exact/norm bonds :

1-2 1-6 1-10 2-3 2-7 3-4 3-8 4-5 4-20 5-6 6-13 7-8 7-9 8-21 10-11  
10-12 13-19 21-22 22-23 22-24 24-58 26-56 27-54 28-53 31-32 31-35 32-33  
33-34 34-35 36-37  
36-40 37-38 38-39 39-40 41-42 41-45 42-43 43-44 44-45

normalized bonds :

25-26 25-30 26-27 27-28 28-29 29-30

G1: [\*1], [\*2]

G2:H,CH3

G3:[\*3],[\*4],[\*5],[\*6],[\*7]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 19:CLASS 20:CLASS 21:CLASS  
22:CLASS 23:CLASS  
24:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom  
33:Atom 34:Atom  
35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom  
44:Atom 45:Atom  
46:CLASS 53:CLASS 54:CLASS 56:CLASS 58:CLASS

L3 178 SEA FILE=REGISTRY SSS FUL L1  
L15 36 SEA FILE=USPATFULL ABB=ON PLU=ON L3  
L16 6627 SEA FILE=USPATFULL ABB=ON PLU=ON ?FLUOROGEN?  
L17 208657 SEA FILE=USPATFULL ABB=ON PLU=ON ?FLUORESCEN?  
L18 267900 SEA FILE=USPATFULL ABB=ON PLU=ON DYE?  
L19 20051 SEA FILE=USPATFULL ABB=ON PLU=ON ?CHROMOPHOR?  
L20 18544 SEA FILE=USPATFULL ABB=ON PLU=ON ?FLUOROPHOR?  
L21 11 SEA FILE=USPATFULL ABB=ON PLU=ON L15 AND (L16 OR L17 OR L18  
OR L19 OR L20)  
L22 5 SEA FILE=USPATFULL ABB=ON PLU=ON (WO2002068678/PN OR  
WO2004090104/PN OR WO2005059163/PN OR WO2005071096/PN OR  
CA2434679/PN OR EP1385853/PN OR EP1616032/PN OR EP1674579/PN  
OR EP1704244/PN OR EP1711504/PN OR JP2005501806/PN OR US2003003  
526/PN OR US2005118669/PN OR US2005181469/PN OR US2005227309/PN  
OR US2005244907/PN OR WO2005024049/PN OR WO2006085978/PN)  
L23 6 SEA FILE=USPATFULL ABB=ON PLU=ON L21 NOT L22

=> dup rem L10 L14 L23

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PROCESSING COMPLETED FOR L10  
PROCESSING COMPLETED FOR L14  
PROCESSING COMPLETED FOR L23

L28 13 DUP REM L10 L14 L23 (1 DUPLICATE REMOVED)  
ANSWERS '1-7' FROM FILE CAPLUS  
ANSWERS '8-13' FROM FILE USPATFULL

=> d ibib abs hitind hitstr L28 1-7; d ibib abs kwic hitstr L28 8-13

L28 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 1  
ACCESSION NUMBER: 2005:474830 CAPLUS Full-text  
DOCUMENT NUMBER: 143:22126  
TITLE: Fluorogenic  $\beta$ -lactamase substrate  
containing a phenolic dye and vinylogous  
cephalosporin, and use for monitoring  $\beta$ -lactamase  
reporter gene expression

INVENTOR(S): Tsien, Roger Y.; Rao, Jianghong  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 40 pp., Cont.-in-part of U.S. Ser. No. 44,486.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

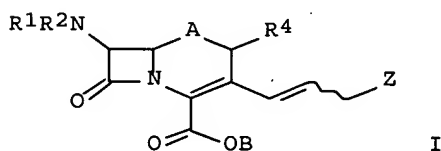
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005118669	A1	20050602	US 2004-884019	20040702
US 2003003526	A1	20030102	US 2002-44486	20020111
US 2005181469	A1	20050818	US 2005-93399	20050329
WO 2006085978	A2	20060817	WO 2005-US23947	20050630

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2001-261313P P 20010112  
 US 2002-44486 A2 20020111  
 US 2004-884019 A 20040702

OTHER SOURCE(S): MARPAT 143:22126  
 GI



AB Provided are *fluorescent* substrates for  $\beta$ -lactamases having the general formula I ( $R_1, R_2 = H, \text{benzyl}, 2\text{-thienylmethyl}, \text{cyanomethyl}$ ;  $B = H, \text{physiol. acceptable salts or metal, ester groups, ammonium cations, } -\text{CHR}_5\text{OCO}(\text{CH}_2)_n\text{CH}_3, -\text{CHR}_5\text{OCOC}(\text{CH}_3)_3, \text{acylthiomethyl}, \text{acyloxy-}\alpha\text{-benzyl}, \delta\text{-butyrolactonyl}, \text{methoxycarbonyloxymethyl}, \text{Ph}, \text{methylsulphinylmethyl}, \delta\text{-morpholinoethyl}, \text{dialkylaminoethyl}, \text{dislkylaminocarbonyloxymethyl}$ ;  $R_4, R_5 = H, \text{lower alkyl}$ ;  $A = S, O, SO, SO_2, CH_2$ ;  $Z = \text{a donor fluorescent moiety that links to the lactam-containing group}$   $n = 0-10$ ). A new class of small *fluorogenic* substrates that work by releasing a phenolate from a vinylogous cephalosporin is reported. The  $\beta$ -lactam ring is cleaved by a  $\beta$ -lactamase enzyme effective to free a fluorophore. Methods of assaying  $\beta$ -lactamase activity and monitoring



expression in systems using beta-lactamase as a reporter gene are also disclosed.

- IC ICM C12Q001-18  
ICS C07D501-14
- INCL 435032000; 540222000
- CC 7-1 (Enzymes)  
Section cross-reference(s): 3
- ST phenolic *dye fluorescent* beta lactamase detn reporter  
gene expression; fluorophore beta lactam ring cleavage lactamase
- IT Flow cytometry  
(FACS (*fluorescence*-activated cell sorting);  
*fluorogenic*  $\beta$ -lactamase substrate containing phenolic  
*dye* and vinylogous cephalosporin, and use for monitoring  
 $\beta$ -lactamase reporter gene expression)
- IT *Dyes*  
Enzyme kinetics  
*Fluorescent* substances  
Fluorometry  
Michaelis constant  
(*fluorogenic*  $\beta$ -lactamase substrate containing phenolic  
*dye* and vinylogous cephalosporin, and use for monitoring  
 $\beta$ -lactamase reporter gene expression)
- IT Reporter gene  
RL: ANT (Analyte); ANST (Analytical study)  
(*fluorogenic*  $\beta$ -lactamase substrate containing phenolic  
*dye* and vinylogous cephalosporin, and use for monitoring  
 $\beta$ -lactamase reporter gene expression)
- IT Phenols, uses  
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
(*fluorogenic*  $\beta$ -lactamase substrate containing phenolic  
*dye* and vinylogous cephalosporin, and use for monitoring  
 $\beta$ -lactamase reporter gene expression)
- IT Animal cell  
(mammalian, reporter gene expression in; *fluorogenic*  
 $\beta$ -lactamase substrate containing phenolic *dye* and vinylogous  
cephalosporin, and use for monitoring  $\beta$ -lactamase reporter gene  
expression)
- IT Ring opening  
(of  $\beta$ -lactam; *fluorogenic*  $\beta$ -lactamase substrate  
containing phenolic *dye* and vinylogous cephalosporin, and use for  
monitoring  $\beta$ -lactamase reporter gene expression)
- IT Biological transport  
(permeation, membrane-permeant  $\beta$ -lactamase substrate;  
*fluorogenic*  $\beta$ -lactamase substrate containing phenolic  
*dye* and vinylogous cephalosporin, and use for monitoring  
 $\beta$ -lactamase reporter gene expression)
- IT Lactams  
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
( $\beta$ -, ring cleavage; *fluorogenic*  $\beta$ -lactamase  
substrate containing phenolic *dye* and vinylogous cephalosporin,  
and use for monitoring  $\beta$ -lactamase reporter gene expression)
- IT Mutagenesis  
( $\beta$ -lactamase; *fluorogenic*  $\beta$ -lactamase substrate  
containing phenolic *dye* and vinylogous cephalosporin, and use for  
monitoring  $\beta$ -lactamase reporter gene expression)
- IT 91-64-5, Coumarin 93-35-6D, Umbelliferone, derivs. 635-78-9, Resorufin  
2321-07-5, Fluorescein

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
(**dye**, substrate containing; **fluorogenic**  
 $\beta$ -lactamase substrate containing phenolic **dye** and vinylogous  
cephalosporin, and use for monitoring  $\beta$ -lactamase reporter gene  
expression)

IT 9073-60-3P

RL: ANT (Analyte); BPN (Biosynthetic preparation); ANST (Analytical  
study); BIOL (Biological study); PREP (Preparation)

(**fluorogenic**  $\beta$ -lactamase substrate containing phenolic  
**dye** and vinylogous cephalosporin, and use for monitoring  
 $\beta$ -lactamase reporter gene expression)

IT 609812-88-6P 852671-27-3P 852671-28-4P  
852671-29-5P

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST  
(Analytical study); PREP (Preparation); USES (Uses)

(**fluorogenic**  $\beta$ -lactamase substrate containing phenolic  
**dye** and vinylogous cephalosporin, and use for monitoring  
 $\beta$ -lactamase reporter gene expression)

IT 93-35-6, 7-Hydroxycoumarin 603-35-0, Triphenylphosphine, reactions  
937-14-4, m-CPBA 7252-83-7 34994-50-8, Resorufin sodium salt  
39098-97-0, 2-Thiopheneacetyl chloride 64308-63-0 79349-53-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of **fluorogenic**  $\beta$ -lactamase substrate;  
**fluorogenic**  $\beta$ -lactamase substrate containing phenolic  
**dye** and vinylogous cephalosporin, and use for monitoring  
 $\beta$ -lactamase reporter gene expression)

IT 16851-02-8P 26748-89-0P 33748-22-0P 70752-63-5P 107550-89-0P  
609812-77-3P 609812-79-5P 609812-80-8P 609812-81-9P 609812-83-1P  
852671-30-8P 852671-32-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(preparation of **fluorogenic**  $\beta$ -lactamase substrate;  
**fluorogenic**  $\beta$ -lactamase substrate containing phenolic  
**dye** and vinylogous cephalosporin, and use for monitoring  
 $\beta$ -lactamase reporter gene expression)

IT 852671-27-3P 852671-28-4P 852671-29-5P

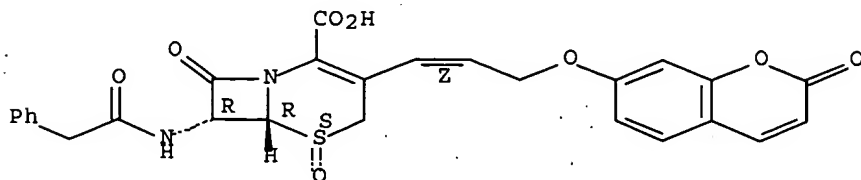
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST  
(Analytical study); PREP (Preparation); USES (Uses)

(**fluorogenic**  $\beta$ -lactamase substrate containing phenolic  
**dye** and vinylogous cephalosporin, and use for monitoring  
 $\beta$ -lactamase reporter gene expression)

RN 852671-27-3 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
8-oxo-3-[(1Z)-3-[(2-oxo-2H-1-benzopyran-7-yl)oxy]-1-propenyl]-7-  
[(phenylacetyl)amino]-, 5-oxide, (5S,6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.

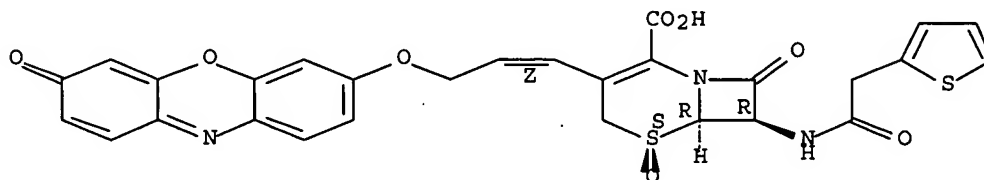


RN 852671-28-4 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
8-oxo-3-[(1Z)-3-[(3-oxo-3H-phenoxazin-7-yl)oxy]-1-propenyl]-7-[(2-thienylacetyl)amino]-, 5-oxide, (5S,6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

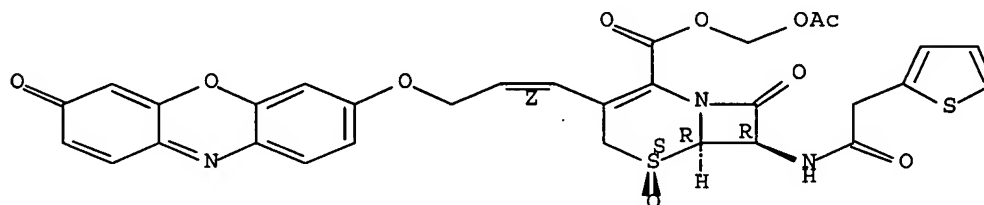


RN 852671-29-5 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
8-oxo-3-[(1Z)-3-[(3-oxo-3H-phenoxazin-7-yl)oxy]-1-propenyl]-7-[(2-thienylacetyl)amino]-, (acetyloxy)methyl ester, 5-oxide, (5S,6R,7R)- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



IT 852671-30-8P 852671-32-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

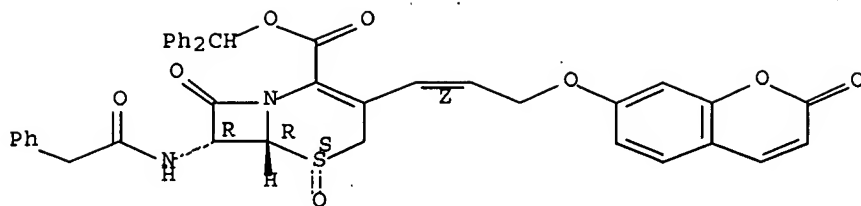
(preparation of *fluorogenic*  $\beta$ -lactamase substrate;  
*fluorogenic*  $\beta$ -lactamase substrate containing phenolic  
dye and vinyllogous cephalosporin, and use for monitoring  
 $\beta$ -lactamase reporter gene expression)

RN 852671-30-8 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
8-oxo-3-[(1Z)-3-[(2-oxo-2H-1-benzopyran-7-yl)oxy]-1-propenyl]-7-  
[(phenylacetyl)amino]-, diphenylmethyl ester, 5-oxide, (5S,6R,7R)- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.

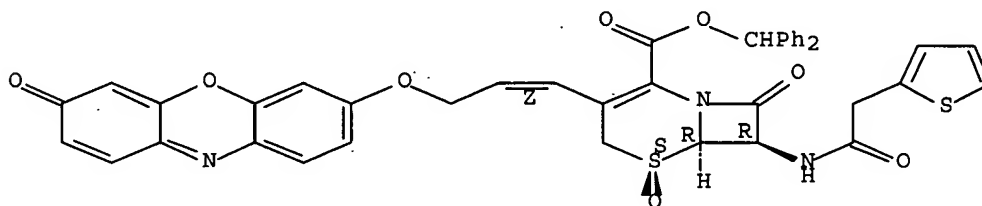
Double bond geometry as shown.



RN 852671-32-0 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
8-oxo-3-[(1Z)-3-[(3-oxo-3H-phenoxazin-7-yl)oxy]-1-propenyl]-7-[(2-thienylacetyl)amino]-, diphenylmethyl ester, 5-oxide, (5S,6R,7R)- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



L28 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:697024 CAPLUS Full-text

DOCUMENT NUMBER: 143:189108

TITLE: *Fluorogenic* substrates for fluorometric

determination of  $\beta$ -lactamase and use for

detection of gene expression and in immunoassay

INVENTOR(S): Corry, Schuyler; Downey, William; Filanoski, Brian;

Gee, Kyle; Greenfield, I. Lawrence; Hirsch, James;

Johnson, Iain; Rukavishnikov, Aleksey;

PATENT ASSIGNEE(S): Molecular Probes, Inc., USA

SOURCE: PCT Int. Appl., 234 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005071096	A2	20050804	WO 2005-US1901	20050121
WO 2005071096	A3	20051215		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, SM

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,  
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,  
EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,  
RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,  
MR, NE, SN, TD, TG

US 2005227309 A1 20051013 US 2005-40924 20050121  
EP 1711504 A2 20061018 EP 2005-711754 20050121

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS

PRIORITY APPLN. INFO.: US 2004-538357P P 20040121  
WO 2005-US1901 W 20050121

OTHER SOURCE(S): MARPAT 143:189108

AB The present invention relates to compds. that are substrates for an enzyme, and upon reaction with the enzyme provide a detectable response, such as an optically detectable response (such as *fluorescence* changes). In particular, the compds. have utility in detecting the presence of a  $\beta$ -lactamase in a sample. The *fluorogenic* substrates of  $\beta$ -lactamase comprise: (a) a  $\beta$ -lactamase substrate moiety, e.g.  $\beta$ -lactam moiety, (b) a first *fluorescent dye* moiety, and (c) a second, optional *fluorescent dye* moiety. Preparation of *fluorogenic* substrates for  $\beta$ -lactamase is reported. In addition to the compds., methods are disclosed for analyzing a sample for the presence of a  $\beta$ -lactamase, for example, as an indicator of expression of a nucleic acid sequence including a sequence coding for a  $\beta$ -lactamase. Kits are disclosed that include the disclosed compds. and addnl. components, for example, cells, antibodies, a  $\beta$ -lactamase or instructions for using the components in an assay, such as an immunoassay (e.g., ELISA).

IC ICM C12Q001-00

CC 7-1 (Enzymes)

Section cross-reference(s): 3, 9, 27, 28

ST fluorometry beta lactamase detn *fluorogenic* substrate gene  
expression immunoassay

IT Antibodies and Immunoglobulins

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
(conjugates; *fluorogenic* substrates for fluorometric determination of  
 $\beta$ -lactamase and use for detection of gene expression and in  
immunoassay)

IT Immunoassay

(enzyme-linked immunosorbent assay; *fluorogenic* substrates  
for fluorometric determination of  $\beta$ -lactamase and use for detection of  
gene expression and in immunoassay)

IT Enzyme immunoassay

Fluorometry

Test kits

(*fluorogenic* substrates for fluorometric determination of  
 $\beta$ -lactamase and use for detection of gene expression and in  
immunoassay)

IT Antigens

RL: ANT (Analyte); ANST (Analytical study)  
(*fluorogenic* substrates for fluorometric determination of  
 $\beta$ -lactamase and use for detection of gene expression and in  
immunoassay)

IT Antibodies and Immunoglobulins

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
(*fluorogenic* substrates for fluorometric determination of  
 $\beta$ -lactamase and use for detection of gene expression and in  
immunoassay)

IT Reporter gene

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)

(*fluorogenic* substrates for fluorometric determination of  $\beta$ -lactamase and use for detection of gene expression and in immunoassay)

IT *Fluorescent dyes*  
*Fluorescent* indicators  
*Fluorescent* substances  
(substrates containing; *fluorogenic* substrates for fluorometric determination of  $\beta$ -lactamase and use for detection of gene expression and in immunoassay)

IT Lactams  
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
( $\beta$ -, substrates containing; *fluorogenic* substrates for fluorometric determination of  $\beta$ -lactamase and use for detection of gene expression and in immunoassay)

IT 9073-60-3  
RL: ANT (Analyte); ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
(*fluorogenic* substrates for fluorometric determination of  $\beta$ -lactamase and use for detection of gene expression and in immunoassay)

IT 861669-38-7P 861669-39-8P 861669-40-1P 861669-41-2P 861669-42-3P  
861669-43-4P 861669-44-5P 861669-45-6P 861669-46-7P 861669-47-8P  
861669-48-9P 861669-49-0P 861669-50-3P 861669-51-4P 861669-52-5P  
861669-53-6P 861669-54-7P 861669-55-8P 861669-56-9P 861669-57-0P  
861669-58-1P 861669-59-2P 861669-61-6P 861669-62-7P 861669-63-8P  
861669-64-9P 861669-66-1P 861669-67-2P 861669-72-9P  
RL: ARG (Analytical reagent use); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation of *fluorogenic* substrates for fluorometric determination of  $\beta$ -lactamase)

IT 861669-60-5P 861669-65-0P 861669-68-3P 861669-69-4P 861669-70-7P  
861669-71-8P 861669-88-7P 861670-03-3P 861670-09-9P  
861670-13-5P 861883-90-1P 861883-93-4P  
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)  
(preparation of *fluorogenic* substrates for fluorometric determination of  $\beta$ -lactamase)

IT 58-71-9 76-54-0, 2',7'-Dichlorofluorescein 90-33-5,  
7-Hydroxy-4-methylcoumarin 99-98-9 100-68-5, Thioanisol 106-95-6,  
Allyl bromide, reactions 118-75-2, Tetrachloro-1,4-benzoquinone,  
reactions 122-59-8, Phenoxycetic acid 303-07-1, 2,6-Dihydroxybenzoic  
acid 635-93-8, 5-Chlorosalicylaldehyde 722-27-0 957-68-6,  
7-Aminocephalosporanic acid 1026-04-6 2321-07-5, Fluorescein  
3163-07-3, 4-Nitroresorcinol 4743-17-3, 5-Chloroisatoic anhydride  
7252-83-7, Bromoacetaldehyde dimethyl acetal 16024-58-1 19766-89-3,  
Sodium 2-ethylhexanoate 28683-92-3 40630-84-0, Allyl bromoacetate  
79349-53-4 104949-45-3 118290-05-4 129393-69-7 165599-63-3  
215868-23-8 861670-07-7 861883-91-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of *fluorogenic* substrates for fluorometric determination of  $\beta$ -lactamase)

IT 5202-85-7P, 5-Chloroanthranilamide 10390-44-0P 101516-66-9P  
115622-74-7P 855946-39-3P 861669-36-5P 861669-37-6P 861669-73-0P  
861669-74-1P 861669-76-3P 861669-77-4P 861669-78-5P 861669-79-6P  
861669-80-9P 861669-81-0P 861669-82-1P 861669-83-2P 861669-84-3P  
861669-85-4P 861669-86-5P 861669-87-6P 861669-89-8P 861669-90-1P  
861669-91-2P 861669-92-3P 861669-93-4P 861669-94-5P 861669-95-6P  
861669-96-7P 861669-97-8P 861669-98-9P 861669-99-0P

861670-00-0P 861670-01-1P 861670-02-2P 861670-04-4P 861670-05-5P  
 861670-06-6P 861670-08-8P 861670-10-2P 861670-11-3P 861670-12-4P  
 861883-89-8P 861883-92-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)

(preparation of *fluorogenic* substrates for fluorometric determination of  
 $\beta$ -lactamase)

IT 233759-98-3P 335193-91-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of *fluorogenic* substrates for fluorometric determination of  
 $\beta$ -lactamase)

IT 861868-25-9 861868-26-0 861868-27-1 861868-28-2 861868-29-3  
 861868-31-7 861868-32-8 861868-33-9 861868-34-0 861868-35-1  
 861868-36-2 861868-37-3 861868-38-4 861868-39-5 861868-40-8  
 861868-41-9 861868-42-0 861868-43-1 861868-44-2 861868-45-3  
 861868-46-4 861868-47-5 861868-48-6 861868-49-7 861868-50-0  
 861868-51-1 861868-52-2 861868-53-3 861868-54-4 861868-55-5  
 861868-56-6 861868-57-7 861868-58-8 861868-59-9 861868-60-2  
 861868-61-3 861868-62-4 861868-63-5 861868-64-6 861868-65-7  
 861868-66-8 861868-67-9 861868-68-0

RL: PRP (Properties)

(unclaimed nucleotide sequence; *fluorogenic* substrates for  
 fluorometric determination of  $\beta$ -lactamase and use for detection of gene  
 expression and in immunoassay)

IT 861868-30-6

RL: PRP (Properties)

(unclaimed protein sequence; *fluorogenic* substrates for  
 fluorometric determination of  $\beta$ -lactamase and use for detection of gene  
 expression and in immunoassay)

IT 292620-73-6 297180-93-9 497257-81-5 636564-46-0 636564-47-1  
 636564-48-2 636564-49-3 636564-51-7 636564-52-8 636564-53-9  
 636564-54-0 636564-55-1 636564-56-2 636564-57-3 636564-58-4  
 636564-59-5 636564-60-8 636564-61-9 636564-62-0 636564-63-1  
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 636565-02-1 636565-03-2 636565-04-3 636565-05-4 636565-06-5  
 636565-07-6 636565-08-7 857248-36-3

RL: PRP (Properties)

(unclaimed sequence; *fluorogenic* substrates for fluorometric  
 determination of  $\beta$ -lactamase and use for detection of gene expression and  
 in immunoassay)

IT 861670-03-3P

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST  
 (Analytical study); PREP (Preparation); USES (Uses)

(preparation of *fluorogenic* substrates for fluorometric determination of  
 $\beta$ -lactamase)

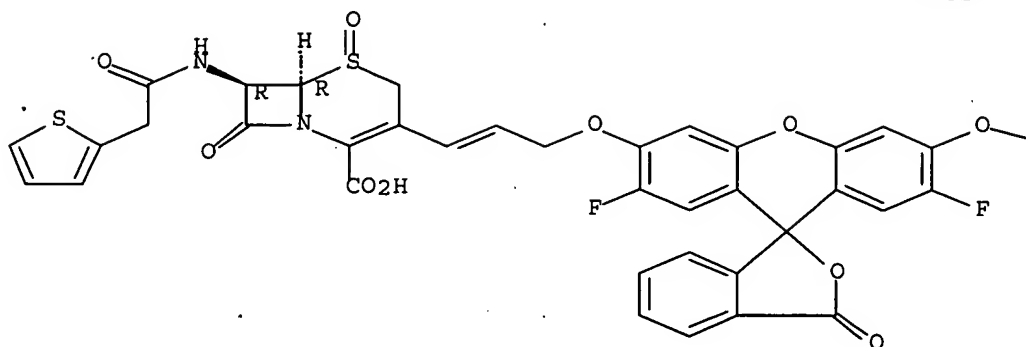
RN 861670-03-3 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
 3,3'-[(2',7'-difluoro-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-  
 3',6'-diyl)bis(oxy-1-propene-3,1-diyl)]bis[8-oxo-7-[(2-  
 thienylacetyl)amino]-, 5,5'-dioxide, (6R,6'R,7R,7'R)- (9CI) (CA INDEX  
 NAME)

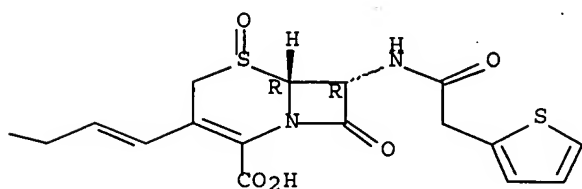
Absolute stereochemistry.

Double bond geometry unknown.

PAGE 1-A



PAGE 1-B



IT 861669-96-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of *fluorogenic* substrates for fluorometric determination of  $\beta$ -lactamase)

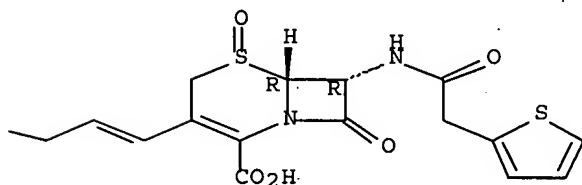
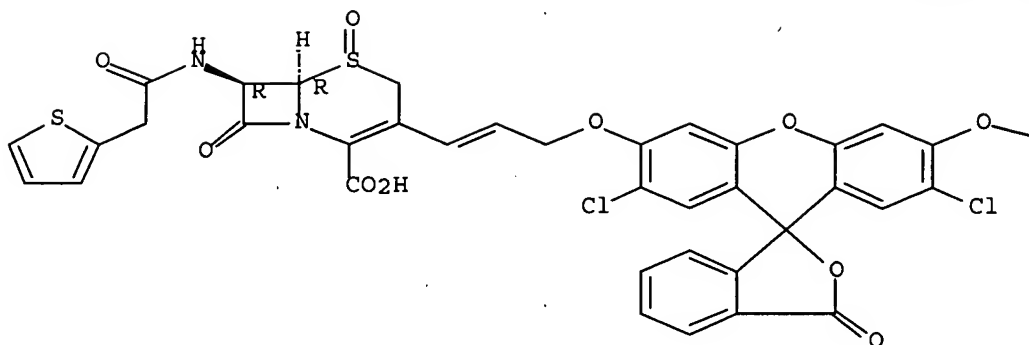
RN 861669-96-7 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3,3'-[(2',7'-dichloro-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-3',6'-diyl)bis(oxy-1-propene-3,1-diyl)]bis[8-oxo-7-[(2-thienylacetyl)amino]-, 5,5'-dioxide, (6R,6'R,7R,7'R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.





L28 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2005:571011 CAPLUS Full-text

DOCUMENT NUMBER: 143:93614

TITLE: In vivo assays for enzyme activity using liposome encapsulating chromogenic substrate to facilitate intracellular delivery

INVENTOR(S): Graham, Ronald J.; Sekar, Michael; Barbisin, Maura

PATENT ASSIGNEE(S): Applera Corporation, USA

SOURCE: PCT Int. Appl., 54 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005059163	A2	20050630	WO 2004-US42639	20041215
WO 2005059163	A3	20051229		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, SM				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,				

RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,  
MR, NE, SN, TD, TG

US 2005244907 A1 20051103 US 2004-14447 20041215  
EP 1704244 A2 20060927 EP 2004-814782 20041215

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS

PRIORITY APPLN. INFO.: US 2003-529953P P 20031215  
US 2004-542425P P 20040206  
WO 2004-US42639 W 20041215

AB The present disclosure relates to methods for detecting an activity of one or more enzymes in a cell. In some embodiments, a cell is contacted with a liposome containing a substrate capable of producing a detectable light signal when acted upon by the enzyme, and detecting the amount of a light signal in the cell, wherein the amount indicates a level of the enzyme activity in the cell. Encapsulation in a liposome facilitates intracellular delivery of substrate. The methods can be used in screening agents that can inhibit or activate an enzyme activity. The methods can also be used in various downstream assays such the detection of interactions between intracellular proteins, screening for variants of an enzyme, and detection of various diseases. Comps. and kits for carrying out the various methods are also provided. These results show that liposomes containing a substrate capable of generating a *fluorescent* signal when acted on by  $\beta$ -galactosidase can be used to detect activity of this enzyme in cells and can be used to determine the presence or absence of this activity in various cell types.

IC ICM C12Q001-00

CC 9-15 (Biochemical Methods)

Section cross-reference(s): 7

IT **Dyes**

(FRET pair, substrate comprises; in vivo assays for enzyme activity using liposome encapsulating chromogenic substrate to facilitate intracellular delivery)

IT **Fluorescence** resonance energy transfer

(dye pair, substrate comprises; in vivo assays for enzyme activity using liposome encapsulating chromogenic substrate to facilitate intracellular delivery)

IT **Microscopy**

(*epifluorescence*, detecting by; in vivo assays for enzyme activity using liposome encapsulating chromogenic substrate to facilitate intracellular delivery)

IT **Microscopes**

(*fluorescence*, detecting by; in vivo assays for enzyme activity using liposome encapsulating chromogenic substrate to facilitate intracellular delivery)

IT **Chemiluminescent substances**

**Fluorescent** indicators

(substrate capable of producing; in vivo assays for enzyme activity using liposome encapsulating chromogenic substrate to facilitate intracellular delivery)

IT **Fluorescent** indicators

( $\beta$ -galactosidyl substituted, substrate capable of producing; in vivo assays for enzyme activity using liposome encapsulating chromogenic substrate to facilitate intracellular delivery)

IT 369-07-3, 2-Nitrophenyl  $\beta$ -D-galactopyranoside 6160-78-7,  
 $\beta$ -Methylumbelliferyl- $\beta$ -D-galactopyranoside 7240-90-6,  
5-Bromo-4-chloro-3-indoyl- $\beta$ -galactopyranoside 17817-20-8,  
Fluorescein di- $\beta$ -D-galactoside 64664-99-9, 3-Carboxyumbelliferyl- $\beta$ -D-galactopyranoside 95079-19-9, Resorufin  $\beta$ -D-galactopyranoside 147963-17-5, 5-Chloromethylfluorescein di- $\beta$ -D-galactopyranoside 183736-52-9, 7-[[[(6-Chloro-7-hydroxy-2-

oxo-2H-1-benzopyran-3-yl)carbonyl]amino]acetyl]amino]-3-[[[3',6'-dihydroxy-3-oxospiro[isobenzofuran-1-(3H),9'-(9H)xanthen]-5-yl]thio]methyl]-8-oxo (6R,7R)-(9CI) 183736-66-5, 7-[[[[[7-[(Acetyloxy)methoxy]-6-chloro-2-oxo-2H-1-benzopyran-3-yl]carbonyl]amino]acetyl]amino]-3-[[[3',6'-bis(acetyloxy)-3-oxospiro[isobenzofuran-1-(3H),9'-(9H)xanthen]-5-yl]thio]methyl]-8-oxo- (acetyloxy)methyl ester (6R,7R)-(9CI) 209540-64-7, 5-(Pentafluorobenzoylamino)fluorescein di-β-D-galactopyranoside 215868-26-1, 6,8-Difluoro-4-methylumbelliferyl β-D-galactopyranoside 452280-31-8 503178-95-8, 9H-(1,3-Dichloro-9,9-dimethylacridin-2-on-7-yl) β-D-galactopyranoside 609812-88-6 609812-89-7, 8-Oxo-3-[3-[(2-oxo-2H-1-benzopyran-7-yl)oxy]-1-propenyl]-7-[(phenylacetyl)amino]-5-oxide (6R,7R)-(9CI) 609812-90-0, 8-Oxo-3-[(1Z)-3-[(3-oxo-3H-phenoxazin-7-yl)oxy]-1-propenyl]-7-[(2-thienylacetyl)amino]-5-oxide (6R,7R)-(9CI)

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (in vivo assays for enzyme activity using liposome encapsulating chromogenic substrate to facilitate intracellular delivery)

IT 452280-31-8 609812-89-7, 8-Oxo-3-[3-[(2-oxo-2H-1-benzopyran-7-yl)oxy]-1-propenyl]-7-[(phenylacetyl)amino]-5-oxide (6R,7R)-(9CI) 609812-90-0, 8-Oxo-3-[(1Z)-3-[(3-oxo-3H-phenoxazin-7-yl)oxy]-1-propenyl]-7-[(2-thienylacetyl)amino]-5-oxide (6R,7R)-(9CI)

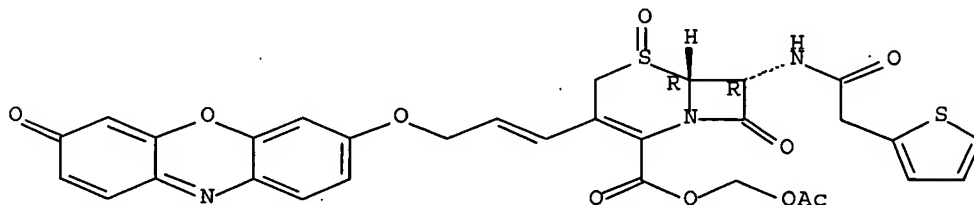
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses) (in vivo assays for enzyme activity using liposome encapsulating chromogenic substrate to facilitate intracellular delivery)

RN 452280-31-8 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 8-oxo-3-[3-[(3-oxo-3H-phenoxazin-7-yl)oxy]-1-propenyl]-7-[(2-thienylacetyl)amino]-, (acetyloxy)methyl ester, 5-oxide, (6R,7R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

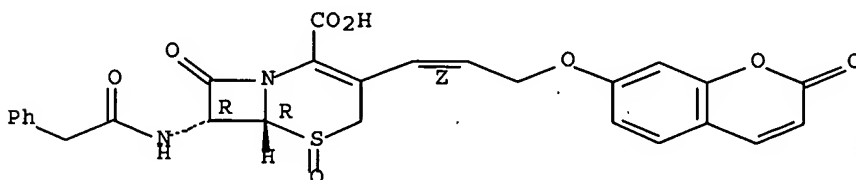


RN 609812-89-7 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 8-oxo-3-[(1Z)-3-[(2-oxo-2H-1-benzopyran-7-yl)oxy]-1-propenyl]-7-[(phenylacetyl)amino]-, 5-oxide, (6R,7R)-(9CI) (CA INDEX NAME)

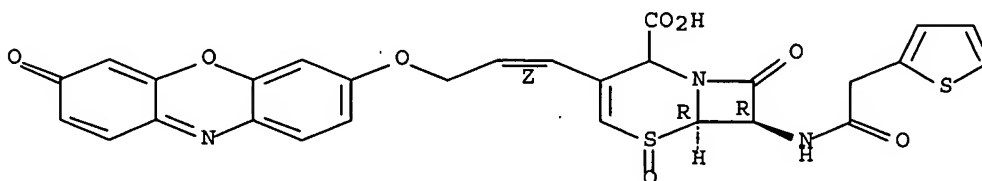
Absolute stereochemistry.

Double bond geometry as shown.



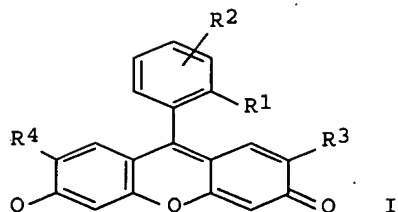
RN 609812-90-0 CAPLUS  
 CN 5-Thia-1-azabicyclo[4.2.0]oct-3-ene-2-carboxylic acid,  
 8-oxo-3-[(1Z)-3-[(3-oxo-3H-phenoxazin-7-yl)oxy]-1-propenyl]-7-[(2-  
 thienylacetyl)amino]-, 5-oxide, (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



L28 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2005:239156 CAPLUS Full-text  
 DOCUMENT NUMBER: 142:312727  
 TITLE: Fluorescent probe used for hydrolase assay  
 INVENTOR(S): Nagano, Tetsuo; Kamiya, Mako; Urano, Yasuteru  
 PATENT ASSIGNEE(S): Daiichi Pure Chemicals Co., Ltd., Japan  
 SOURCE: PCT Int. Appl., 54 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005024049	A1	20050317	WO 2004-JP13185	20040903
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1674579	A1	20060628	EP 2004-772924	20040903
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
PRIORITY APPLN. INFO.:			JP 2003-314041	A 20030905
			WO 2004-JP13185	W 20040903
OTHER SOURCE(S):			MARPAT 142:312727	
GI				



- AB A novel *fluorescent* probe is provided, which is represented by the following formula (I), and is utilized for a *fluorescence* assay of a hydrolase. In the formula I, R1 represents a hydrogen atom, a carboxy group or a monovalent substituent other than a sulfonate group; R2 represents a hydrogen atom or a monovalent substituent; R3 and R4 each independently represents a hydrogen atom or a halogen atom; and R5 represents a monovalent group which is cleaved upon contact with a substance to be detected; provided that the combination of R1 and R2 is selected so that the benzene ring to which R1 and R2 are bound has such an oxidation potential that (1) the compound I has substantially no *fluorescence* before the cleavage; and (2) the resultant compound formed from I by the cleavage is substantially highly *fluorescent* after the cleavage.
- IC ICM C12Q001-34  
ICS G01N021-64; G01N021-78
- CC 9-5 (Biochemical Methods)
- ST *fluorescent* probe oxidn potential bond cleavage hydrolase assay
- IT Bond cleavage  
    *Fluorescent* indicators  
    Fluorometry  
    Hydrolysis  
    Oxidation potential  
        (*fluorescent* probe capable of generating *fluorescence* upon bond cleavage in hydrolase assay)
- IT Electron transfer  
    (photochem.; *fluorescent* probe capable of generating *fluorescence* upon bond cleavage in hydrolase assay)
- IT Functional groups  
    ( $\beta$ -galactopyranosyl, cyclic amide; *fluorescent* probe capable of generating *fluorescence* upon bond cleavage in hydrolase assay)
- IT 9027-41-2, Hydrolase  
    RL: ANT (Analyte); ANST (Analytical study)  
        (and carbohydrate-hydrolyzing; *fluorescent* probe capable of generating *fluorescence* upon bond cleavage in hydrolase assay)
- IT 9073-60-3  
    RL: ANT (Analyte); ANST (Analytical study)  
        (*fluorescent* probe capable of generating *fluorescence* upon bond cleavage in hydrolase assay)
- IT 9001-78-9 9031-11-2,  $\beta$ -Galactosidase  
    RL: ANT (Analyte); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)  
        (*fluorescent* probe capable of generating *fluorescence* upon bond cleavage in hydrolase assay)
- IT 847978-23-8P 847978-28-3P 847978-50-1P 847978-57-8P  
    RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)

(fluorescent probe capable of generating fluorescence upon bond cleavage in hydrolase assay)

IT 95-46-5, 2-Bromotoluene 96-32-2, Methylbromoacetate 603-35-0, Triphenylphosphine, reactions 814-49-3, Diethylchlorophosphate 937-14-4, m-Chloroperbenzoic acid 1214-24-0 7252-83-7, 2-Bromo-1,1-dimethoxyethane 7681-82-5, Sodiumiodide, reactions 14472-14-1, 4-Bromo-3-methylphenol 16029-98-4, Iodotrimethylsilane 18162-48-6, tert-Butyldimethylsilylchloride 19285-38-2 104146-10-3 121714-18-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(fluorescent probe capable of generating fluorescence upon bond cleavage in hydrolase assay)

IT 590-97-6P 5454-83-1P 119636-62-3P 169315-83-7P 643755-80-0P 643755-81-1P 643755-82-2P 643755-83-3P 643755-84-4P 643755-85-5P 643755-86-6P 643755-87-7P 847978-25-0P 847978-34-1P 847978-36-3P 847978-38-5P 847978-45-4P 847978-47-6P 847978-52-3P 847978-54-5P 847978-55-6P 847978-56-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(fluorescent probe capable of generating fluorescence upon bond cleavage in hydrolase assay)

IT 847978-41-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(fluorescent probe capable of generating fluorescence upon bond cleavage in hydrolase assay)

IT 9013-79-0, Esterase

RL: ANT (Analyte); ANST (Analytical study)

(phosphoric acid ester; fluorescent probe capable of generating fluorescence upon bond cleavage in hydrolase assay)

IT 847978-57-8P

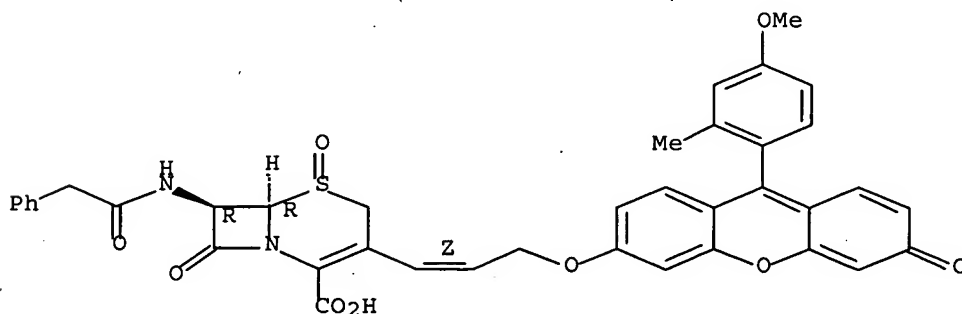
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)

(fluorescent probe capable of generating fluorescence upon bond cleavage in hydrolase assay)

RN 847978-57-8 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[1Z]-3-[[9-(4-methoxy-2-methylphenyl)-3-oxo-3H-xanthen-6-yl]oxy]-1-propenyl]-8-oxo-7-[(phenylacetyl)amino]-, 5-oxide, (6R,7R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



IT 847978-56-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

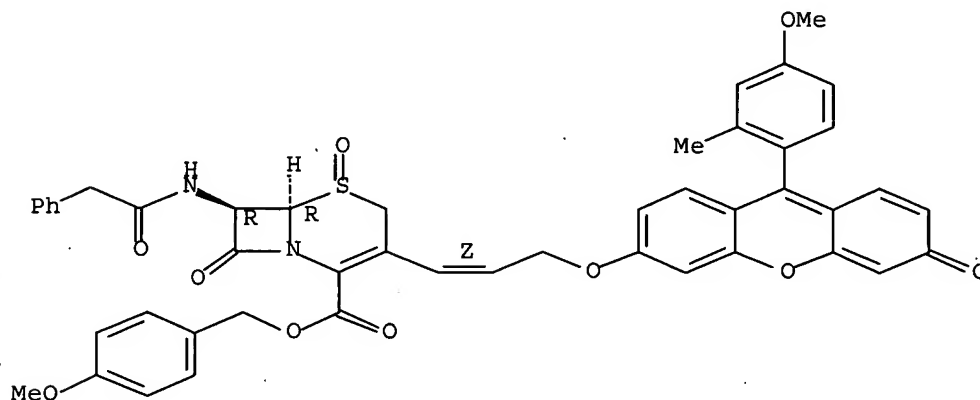
(*fluorescent* probe capable of generating *fluorescence* upon bond cleavage in hydrolase assay)

RN 847978-56-7 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 3-[[1Z]-3-[[9-(4-methoxy-2-methylphenyl)-3-oxo-3H-xanthen-6-yl]oxy]-1-propenyl]-8-oxo-7-[(phenylacetyl)amino]-, (4-methoxyphenyl)methyl ester, 5-oxide, (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:878473 CAPLUS Full-text

DOCUMENT NUMBER: 141:389858

TITLE: reporting system for monitoring real-time gene expression events in live cells using *fluorogenic* substrates

INVENTOR(S): Xie, X. Sunney; Xiao, Jie; Cai, Long; Markson, Joseph Scott; Yu, Ji; Yin, Jialu

PATENT ASSIGNEE(S): President and Fellows of Harvard College, USA; Regents of the University of California

SOURCE: PCT Int. Appl., 69 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004090104	A2	20041021	WO 2004-US10341	20040402
WO 2004090104	A3	20050303		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,

TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,  
BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,  
ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,  
SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,  
TD, TG

EP 1616032 A2 20060118 EP 2004-749716 20040402

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR

PRIORITY APPLN. INFO.: US 2003-459897P P 20030402

WO 2004-US10341 W 20040402

AB The current invention provides a reporting system for monitoring real-time gene expression events in live cells using *fluorogenic* substrates. Modified  $\beta$ -galactosidase,  $\beta$ -glucosidase,  $\beta$ -lactamase with short maturation time and a short cellular lifetime are selected as reporter to detect transient gene expression event in live cells. Gene expression signals are monitored by visible and UV spectrometry, and fluorometry.

IC ICM C12N

CC 3-3 (Biochemical Genetics)

Section cross-reference(s): 7, 10

ST sequence Escherichia ubiquitin beta galactosidase lacZ; yellow *fluorescent* protein gene sequence; live cell gene expression reporting system

IT DNA sequences

(for modified ubiquitin fusion  $\beta$ -galactosidase (E. coli) lacZ and yellow *fluorescent* protein gene)

IT Protein sequences

(for modified ubiquitin fusion  $\beta$ -galactosidase (Escherichia coli) and yellow *fluorescent* protein)

IT Escherichia coli

Saccharomyces cerevisiae

Shewanella oneidensis

(gene expression at; reporting system for monitoring real-time gene expression events in live cells using *fluorogenic* substrates)

IT Gene, microbial

RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)

(lacZ; reporting system for monitoring real-time gene expression events in live cells using *fluorogenic* substrates)

IT Fluorometry

UV and visible spectroscopy

(reporting system for monitoring real-time gene expression events in live cells using *fluorogenic* substrates)

IT Gene, animal

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(ssrA; reporting system for monitoring real-time gene expression events in live cells using *fluorogenic* substrates)

IT Proteins

RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); USES (Uses)

(yellow *fluorescent*; reporting system for monitoring real-time gene expression events in live cells using *fluorogenic* substrates)

IT 183736-52-9, CCF 2

RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)

(CCF 2; reporting system for monitoring real-time gene expression



events in live cells using *fluorogenic* substrates)

IT 452280-30-7, CR 2  
 RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (CR 2; reporting system for monitoring real-time gene expression events in live cells using *fluorogenic* substrates)

IT 784214-83-1  
 RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (amino acid sequence; reporting system for monitoring real-time gene expression events in live cells using *fluorogenic* substrates)

IT 776338-24-0 776338-26-2 776338-28-4 784214-78-4 784214-80-8 784214-82-0  
 RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (amino acid sequence; reporting system for monitoring real-time gene expression events in live cells using *fluorogenic* substrates)

IT 776338-29-5, DNA (plasmid pVS5 gene Venus-ssrA)  
 RL: ARG (Analytical reagent use); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (nucleotide sequence; reporting system for monitoring real-time gene expression events in live cells using *fluorogenic* substrates)

IT 776338-23-9 776338-25-1 776338-27-3 784214-77-3 784214-79-5 784214-81-9  
 RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (nucleotide sequence; reporting system for monitoring real-time gene expression events in live cells using *fluorogenic* substrates)

IT 60267-61-0, Ubiquitin  
 RL: BSU (Biological study, unclassified); BIOL (Biological study)  
 (reporter protein fusion with; reporting system for monitoring real-time gene expression events in live cells using *fluorogenic* substrates)

IT 9001-22-3,  $\beta$ -Glucosidase 9031-11-2,  $\beta$ -Galactosidase 9073-60-3,  $\beta$ -Lactamase  
 RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (reporter; reporting system for monitoring real-time gene expression events in live cells using *fluorogenic* substrates)

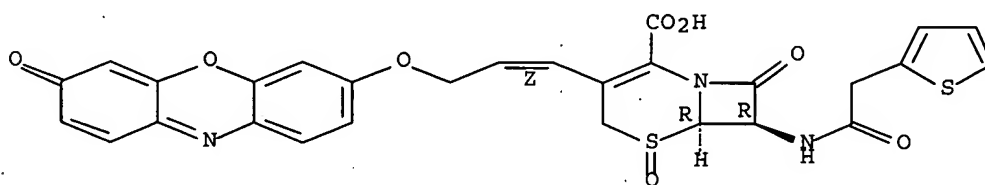
IT 776318-68-4  
 RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (ssrA peptide sequence; reporting system for monitoring real-time gene expression events in live cells using *fluorogenic* substrates)

IT 95079-19-9 101490-85-1 503178-95-8 776318-69-5  
 RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (substrate; reporting system for monitoring real-time gene expression events in live cells using *fluorogenic* substrates)

IT 776782-40-2 776782-41-3 776782-42-4 776782-43-5 776782-44-6 776782-45-7  
 RL: PRP (Properties)  
 (unclaimed nucleotide sequence; reporting system for monitoring real-time gene expression events in live cells using *fluorogenic* substrates)

IT 776782-46-8 776782-47-9 776782-48-0 776782-49-1 776782-50-4  
 776782-51-5  
 RL: PRP (Properties)  
 (unclaimed sequence; reporting system for monitoring real-time gene  
 expression events in live cells using *fluorogenic* substrates)  
 IT 452280-30-7, CR 2  
 RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); ANST  
 (Analytical study); BIOL (Biological study); USES (Uses)  
 (CR 2; reporting system for monitoring real-time gene expression events  
 in live cells using *fluorogenic* substrates)  
 RN 452280-30-7 CAPLUS  
 CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
 8-oxo-3-[(1Z)-3-[(3-oxo-3H-phenoxazin-7-yl)oxy]-1-propenyl]-7-[(2-  
 thienylacetyl)amino]-, 5-oxide, (6R,7R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



L28 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2003:643607 CAPLUS Full-text  
 DOCUMENT NUMBER: 139:287990  
 TITLE: Novel *Fluorogenic* Substrates for Imaging  
 $\beta$ -Lactamase Gene Expression  
 AUTHOR(S): Gao, Wenzhong; Xing, Bengang; Tsien, Roger Y.; Rao,  
 Jianghong  
 CORPORATE SOURCE: Department of Molecular and Medical Pharmacology,  
 Crump Institute for Molecular Imaging, University of  
 California, Los Angeles, CA, 90095-1770, USA  
 SOURCE: Journal of the American Chemical Society (2003),  
 125(37), 11146-11147  
 CODEN: JACSAT; ISSN: 0002-7863  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 139:287990  
 AB A new class of small *nonfluorescent fluorogenic* substrates, based on release  
 of a phenolic *dye* from a vinylogous cephalosporin, becomes brightly  
*fluorescent* after  $\beta$ -lactamase hydrolysis with up to 153-fold enhancement in  
 the *fluorescence* intensity. Less than 500 fM of  $\beta$ -lactamase in cell lysates  
 can be readily detected, and  $\beta$ -lactamase expression in living cells can be  
 imaged with a red *fluorescence* derivative These new *fluorogenic* substrates  
 should find uses in clin. diagnostics and facilitate the applications of  $\beta$ -  
 lactamase as a biosensor.  
 CC 7-1 (Enzymes)  
 Section cross-reference(s): 26  
 ST vinylogous cephalosporin prepn *fluorogenic* imaging lactamase  
 detection  
 IT 9073-60-3,  $\beta$ -Lactamase

RL: ANT (Analyte); ANST (Analytical study)

(preparation of vinyllogous cephalosporin *fluorogenic* substrates  
and use for detection of  $\beta$ -lactamase)

IT 609812-88-6P 609812-89-7P 609812-90-0P  
609812-91-1P

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST  
(Analytical study); PREP (Preparation); USES (Uses)

(preparation of vinyllogous cephalosporin *fluorogenic* substrates  
and use for detection of  $\beta$ -lactamase)

IT 93-35-6, 7-Hydroxycoumarin 7252-83-7 34994-50-8, Resorufin sodium salt  
39098-97-0, 2-Thiopheneacetyl chloride 64308-63-0 79349-53-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of vinyllogous cephalosporin *fluorogenic* substrates  
and use for detection of  $\beta$ -lactamase)

IT 704884-54-8 16851-02-8P 26748-89-0P 33748-22-0P 70752-63-5P  
107550-89-0P 609812-77-3P 609812-78-4P 609812-79-5P  
609812-80-8P 609812-81-9P 609812-82-0P 609812-83-1P  
609812-84-2P 609812-85-3P 609812-86-4P 609812-87-5P

RL: RCT (Reactant); SPN (Synthetic preparation)

(preparation of vinyllogous cephalosporin *fluorogenic* substrates  
and use for detection of  $\beta$ -lactamase)

IT 609812-89-7P 609812-90-0P 609812-91-1P

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST  
(Analytical study); PREP (Preparation); USES (Uses)

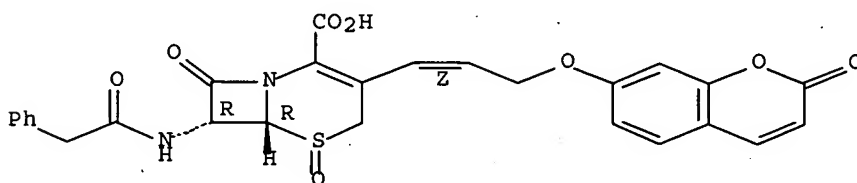
(preparation of vinyllogous cephalosporin *fluorogenic* substrates  
and use for detection of  $\beta$ -lactamase)

RN 609812-89-7 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
8-oxo-3-[(1Z)-3-[(2-oxo-2H-1-benzopyran-7-yl)oxy]-1-propenyl]-7-  
[(phenylacetyl)amino]-, 5-oxide, (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

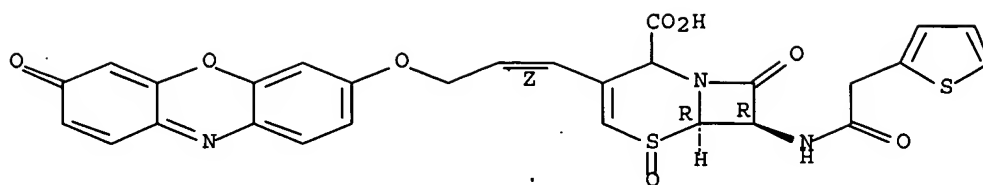


RN 609812-90-0 CAPLUS

CN 5-Thia-1-azabicyclo[4.2.0]oct-3-ene-2-carboxylic acid,  
8-oxo-3-[(1Z)-3-[(3-oxo-3H-phenoxazin-7-yl)oxy]-1-propenyl]-7-[(2-  
thienylacetyl)amino]-, 5-oxide, (6R,7R)- (9CI) (CA INDEX NAME)

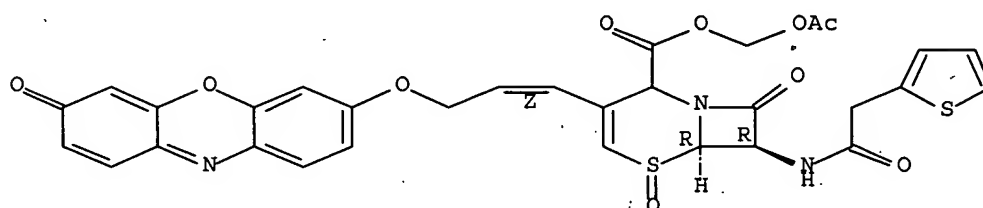
Absolute stereochemistry.

Double bond geometry as shown.



RN 609812-91-1 CAPLUS  
 CN 5-Thia-1-azabicyclo[4.2.0]oct-3-ene-2-carboxylic acid,  
 8-oxo-3-[(1Z)-3-[(3-oxo-3H-phenoxazin-7-yl)oxy]-1-propenyl]-7-[(2-  
 thienylacetyl)amino]-, (acetyloxy)methyl ester, 5-oxide, (6R,7R)- (9CI)  
 (CA INDEX NAME)

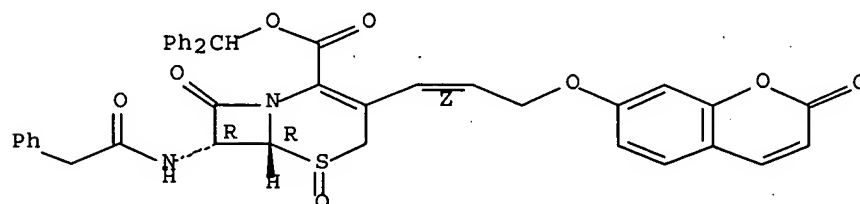
Absolute stereochemistry.  
 Double bond geometry as shown.



IT 609812-78-4P 609812-82-0P 609812-85-3P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of vinylogous cephalosporin *fluorogenic* substrates  
 and use for detection of  $\beta$ -lactamase)

RN 609812-78-4 CAPLUS  
 CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
 8-oxo-3-[(1Z)-3-[(2-oxo-2H-1-benzopyran-7-yl)oxy]-1-propenyl]-7-  
 [(phenylacetyl)amino]-, diphenylmethyl ester, 5-oxide, (6R,7R)- (9CI) (CA  
 INDEX NAME)

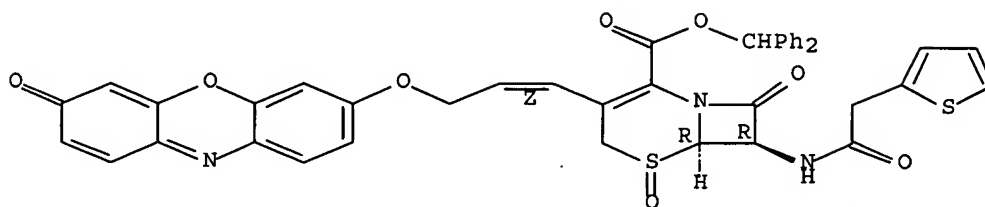
Absolute stereochemistry.  
 Double bond geometry as shown.



RN 609812-82-0 CAPLUS  
 CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
 8-oxo-3-[(1Z)-3-[(3-oxo-3H-phenoxazin-7-yl)oxy]-1-propenyl]-7-[(2-

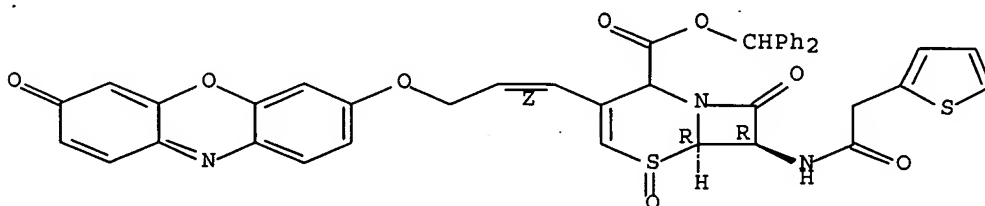
thienylacetyl)amino]-, diphenylmethyl ester, 5-oxide, (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



RN 609812-85-3 CAPLUS  
CN 5-Thia-1-azabicyclo[4.2.0]oct-3-ene-2-carboxylic acid,  
8-oxo-3-[(1Z)-3-[(3-oxo-3H-phenoxazin-7-yl)oxy]-1-propenyl]-7-[(2-thienylacetyl)amino]-, diphenylmethyl ester, 5-oxide, (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



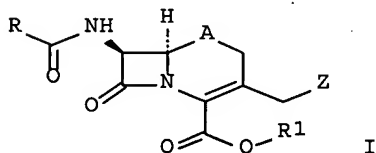
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 2002:676218 CAPLUS Full-text  
DOCUMENT NUMBER: 137:197525  
TITLE:  $\beta$ -Lactamase substrates having phenolic ethers and their use for  $\beta$ -lactamase determination  
INVENTOR(S): Tsien, Roger Y.; Rao, Jianghong  
PATENT ASSIGNEE(S): The Regents of the University of California, USA  
SOURCE: PCT Int. Appl., 46 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002068678	A2	20020906	WO 2002-US769	20020111
WO 2002068678	A3	20031204		

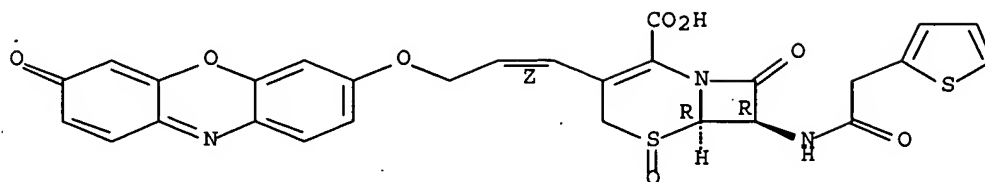
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,  
 GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,  
 LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,  
 PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,  
 UA, UG, US, UZ, VN, YU, ZA, ZM, ZW  
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,  
 KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB,  
 GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA,  
 GN, GQ, GW, ML, MR, NE, SN, TD, TG  
 CA 2434679 AA 20020906 CA 2002-2434679 20020111  
 EP 1385853 A2 20040204 EP 2002-720779 20020111  
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
 IE, SI, LT, LV, FI, RO, MK, CY, AL, TR  
 JP 2005501806 T2 20050120 JP 2002-568772 20020111  
 PRIORITY APPLN. INFO.: US 2001-261313P P 20010112  
 WO 2002-US769 W 20020111  
 OTHER SOURCE(S): MARPAT 137:197525  
 GI



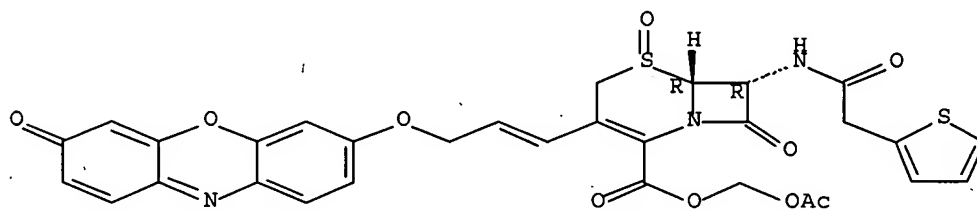
AB Provided are *fluorescent*  $\beta$ -lactamase substrates I (R = benzyl, 2-thienylmethyl, cyanomethyl; R1 = H, physiol. acceptable salts or metal, ester groups, ammonium cations, --CHR2OCO(CH2)nCH3, --CHR2OCOC(CH3)3, acylthiomethyl, acyloxy- $\alpha$ -benzyl,  $\delta$ -butyrolactonyl, methoxycarbonyloxymethyl, Ph, methylsulphinylmethyl,  $\beta$ -morpholinoethyl, dialkylaminoethyl, disalkylaminocarbonyloxymethyl; R2 = H, lower alkyl; A = S, O, SO, SO2, CH2; Z = a donor *fluorescent* moiety). Also provided are methods of use of these compds. for  $\beta$ -lactamase determination  
 IC ICM C12Q  
 CC 7-3 (Enzymes)  
 IT 452280-29-4P 452280-30-7P 452280-31-8P 452280-32-9P  
 RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)  
 ( $\beta$ -Lactamase substrates having phenolic ethers and their use for  $\beta$ -lactamase determination)  
 IT 452280-30-7P 452280-31-8P 452280-32-9P  
 RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)  
 ( $\beta$ -Lactamase substrates having phenolic ethers and their use for  $\beta$ -lactamase determination)  
 RN 452280-30-7 CAPLUS  
 CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 8-oxo-3-[(1Z)-3-[(3-oxo-3H-phenoxazin-7-yl)oxy]-1-propenyl]-7-[(2-thienylacetyl)amino]-, 5-oxide, (6R,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



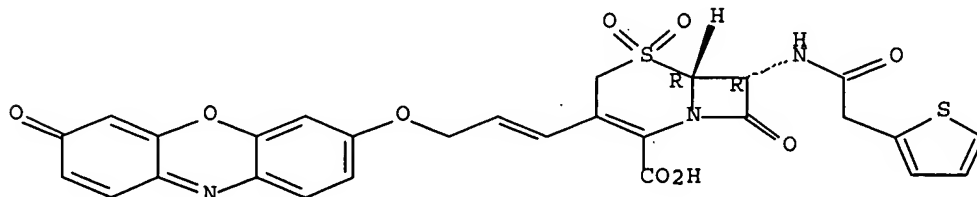
RN 452280-31-8 CAPLUS  
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
8-oxo-3-[3-[(3-oxo-3H-phenoxazin-7-yl)oxy]-1-propenyl]-7-[(2-  
thienylacetyl)amino]-, (acetyloxy)methyl ester, 5-oxide, (6R,7R) - (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry unknown.



RN 452280-32-9 CAPLUS  
CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
8-oxo-3-[3-[(3-oxo-3H-phenoxazin-7-yl)oxy]-1-propenyl]-7-[(2-  
thienylacetyl)amino]-, 5,5-dioxide, (6R,7R) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry unknown.



L28 ANSWER 8 OF 13 USPATFULL on STN  
ACCESSION NUMBER: 81:6597 USPATFULL Full-text  
TITLE: Cephem carbonylmethyl derivatives

INVENTOR(S): Scartazzini, Riccardo, Allschwil, Switzerland  
Bickel, Hans, Binningen, Switzerland  
PATENT ASSIGNEE(S): Ciba-Geigy Corporation, Ardsley, NY, United States  
(U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 4248868		19810203
APPLICATION INFO.:	US 1979-14454		19790223 (6)
RELATED APPLN. INFO.:	Continuation of Ser. No. US 1976-715084, filed on 17 Aug 1976, now abandoned		

	NUMBER	DATE
PRIORITY INFORMATION:	CH 1975-10904	19750822
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	Granted	
PRIMARY EXAMINER:	Rizzo, Nicholas S.	
LEGAL REPRESENTATIVE:	Almaula, Prabodh I.	
NUMBER OF CLAIMS:	23	
EXEMPLARY CLAIM:	1	
LINE COUNT:	2607	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention comprises carbonylmethyl derivatives of the formula IA and corresponding carbonylmethylene derivatives of the formula IB ##STR1## in which R.sub.1.sup.a represents a member of the group comprising hydrogen and an acyl radical of the formula A

R.sub.a --C(R.sub.b)(R.sub.c)--C(.dbd.O)-- (A)

in which R.sub.a represents a member of the group comprising optionally substituted phenyl, thienyl, furyl, cyclohexadienyl and cyclohexenyl, R.sub.b represents hydrogen and R.sub.c represents a member of the group comprising hydrogen, optionally protected hydroxyl, optionally protected amino and phenyl-lower protected sulpho, or in which R.sub.a represents a member of the group comprising cyano, optionally substituted phenoxy, pyridylthio, and tetrazolyl, and R.sub.b and R.sub.c each represent hydrogen, or in which R.sub.a represents a member of the group comprising phenyl, thienyl, furyl, and R.sub.b and R.sub.c together denote a member of the group comprising lower alkoxyimino, cycloalkoxyimino and phenyl-lower alkoxyimino in the syn-configuration, and such a group of the formula (A) contains at most one free amino group, R.sub.1.sup.b represents hydrogen, R.sub.2 represents a member of the group comprising hydroxyl,  $\alpha$ -poly-branched lower alkoxy and 2-halogeno-lower alkoxy, which can easily be converted into the latter, and also phenacyloxy, 1-phenyl-lower alkoxy which has 1-3 phenyl radicals which are optionally substituted by lower alkoxy or nitro, lower alkanoyloxymethoxy,  $\alpha$ -amino-lower alkanoyloxymethoxy, or 2-phthalidyloxy, and also tris-lower alkylsilyloxy, and R.sub.3 represents a member of the group comprising hydrogen, lower alkyl, cycloalkyl, phenyl which is optionally substituted by lower alkyl, lower alkoxy or halogen, phenyl-lower alkyl which is optionally substituted by nitro, lower alkyl, lower alkoxy or halogen, hydroxyl, etherified hydroxyl, especially lower alkoxy, above all methoxy, amino, lower alkylamino, di-lower alkylamino, lower alkyleneamino, oxa-lower alkyleneamino, phenylamino, hydroxylamino, lower alkoxyamino, hydrazino, 2-lower alkylhydrazino, 2-phenylhydrazino, 4-lower alkylpiperazin-1-ylamino, lower alkylamino which is substituted by amino and/or carboxyl, and heterocyclylamino which is optionally substituted by lower alkyl, and wherein the heterocyclyl radical preferably contains 5-6



rings members and contains, as hetero-atoms, nitrogen, which is optionally also in the N-oxidized form, oxygen or sulphur and 1-oxides and salts of such compounds, which compounds are active against microorganisms, such as Gram-positive and Gram-negative bacteria, and pharmaceutical preparations containing these compounds.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

SUMM . . . agents, for example starches, agar, alginic acid or a salt thereof, such as sodium alginate, and/or effervescent mixtures, or adsorbents, *dyestuffs*, flavouring substances and sweeteners. Furthermore, the new pharmacologically active compounds can be used in the form of injectable formulations, for. . .

IT 63760-38-3P 63760-42-9P 63760-50-9P  
63760-68-9P

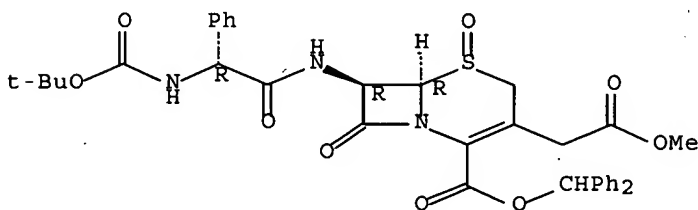
(preparation and reduction of)

IT 63760-38-3P 63760-42-9P 63760-50-9P  
(preparation and reduction of)

RN 63760-38-3 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-3-acetic acid, 7-[[[(1,1-dimethylethoxy) carbonyl] amino] phenylacetyl] amino]-2-[(diphenylmethoxy) carbonyl]-8-oxo-, methyl ester, 5-oxide, [6R-[6 $\alpha$ ,7 $\beta$ (R\*)]]- (9CI) (CA INDEX NAME)

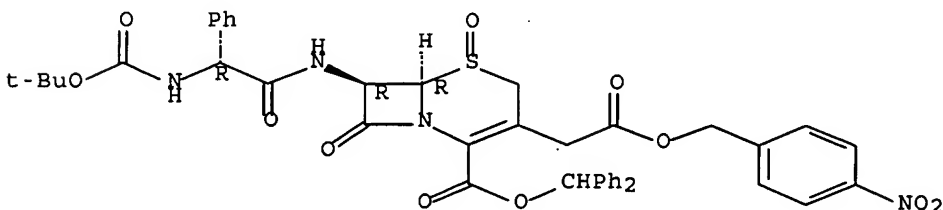
Absolute stereochemistry.



RN 63760-42-9 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-3-acetic acid, 7-[[[(1,1-dimethylethoxy) carbonyl] amino] phenylacetyl] amino]-2-[(diphenylmethoxy) carbonyl]-8-oxo-, (4-nitrophenyl) methyl ester, 5-oxide, [6R-[6 $\alpha$ ,7 $\beta$ (R\*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

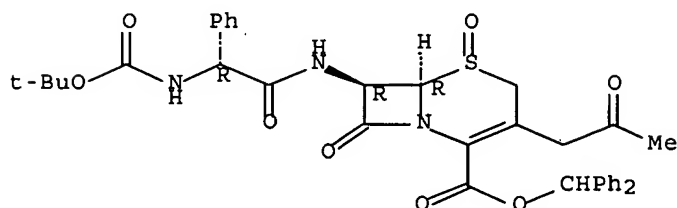


RN 63760-50-9 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[[[(1,1-dimethylethoxy) carbonyl] amino] phenylacetyl] amino]-8-oxo-3-(2-

oxopropyl)-, diphenylmethyl ester, 5-oxide, [6R-[6 $\alpha$ ,7 $\beta$ (R\*)]]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L28 ANSWER 9 OF 13 USPATFULL on STN

ACCESSION NUMBER: 78:50766 USPATFULL Full-text

TITLE: Preparation of cephalosporin compounds

INVENTOR(S): Laundon, Brian, Northolt, Great Britain

Cowley, Brian Richard, Greenford, Great Britain

Humber, David Cedric, London, Great Britain

PATENT ASSIGNEE(S): Glaxo Laboratories Limited, Greenford, Great Britain  
(non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 4113591		19780912
APPLICATION INFO.:	US 1976-749300		19761210 (5)
RELATED APPLN. INFO.:	Continuation of Ser. No. US 1975-593273, filed on 7 Jul 1975, now abandoned which is a continuation of Ser. No. US 1974-455073, filed on 27 Mar 1974, now abandoned which is a continuation of Ser. No. US 1972-306308, filed on 14 Nov 1972, now abandoned which is a division of Ser. No. US 1970-66128, filed on 21 Aug. 1970, now abandoned		

	NUMBER	DATE
PRIORITY INFORMATION:	GB 1969-42502	19690826
	GB 1970-14980	19700326
	GB 1970-3463	19700123
	GB 1970-33698	19700710

DOCUMENT TYPE: Utility

FILE SEGMENT: Granted

PRIMARY EXAMINER: Williams, Howard S.

LEGAL REPRESENTATIVE: Bacon & Thomas

NUMBER OF CLAIMS: 4

EXEMPLARY CLAIM: 1

LINE COUNT: 4100

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention relates to a novel method for the preparation of a 7 $\beta$ -acylamido-3-bromomethylceph-3-em-4-carboxylic acid-1-oxide compound by brominating a 7 $\beta$ -acylamido-3-methylceph-3-em-4-carboxylic acid-1-oxide compound.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

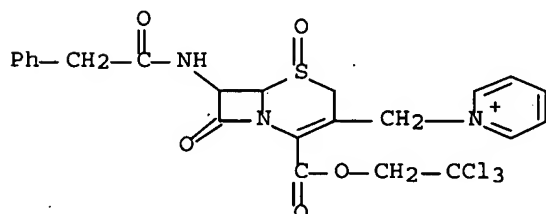
DETD . . . 20 mmole) in dry, ethanol-free chloroform (300 ml.) was heated to reflux in an atmosphere of nitrogen, and illuminated by **fluorescent** strip-lighting (8 + 40-watt lamps). N-Bromosuccinimide (890 mg., 5 mmole) was added and the mixture refluxed for 13/4hr., further portions. . .

DETD . . . 10.4 mmole) in benzene (500 ml.) was stirred and heated to reflux in an atmosphere of nitrogen, and illuminated with **fluorescent** strip-lighting (8 + 40-watt lamps). N-Bromosuccinimide (3 g., 16.85 mmole) was added and the mixture refluxed for 30 minutes, then. . .

DETD . . . heated under reflux for 1 hour in a stream of dry nitrogen while being illuminated by 8 + 40 watt **fluorescent** strip-lights. The reaction mixture was filtered from a trace of insoluble material and the benzene was evaporated. The residue was. . .

DETD . . . heated under reflux for 1 hour in a stream of dry nitrogen while being illuminated by 8 + 40 watt **fluorescent** strip-lights. The benzene was removed in vacuo and the residual orange foam was chromatographed on Kieselgel G (150 g) with. . .

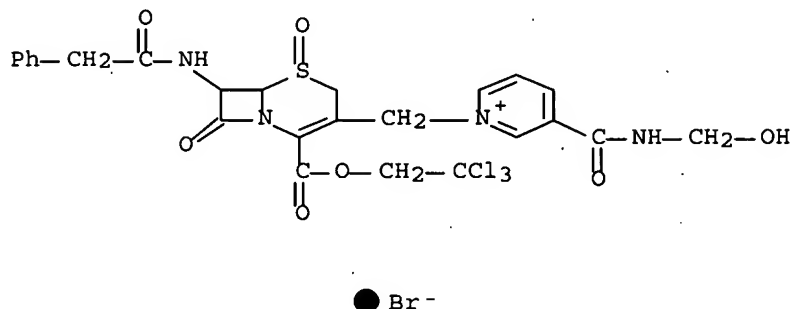
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 33247-54-0P 33247-55-1P 33247-56-2P 33465-36-0P 33465-37-1P  
 33465-38-2P 33465-39-3P 33465-40-6P 33465-41-7P 33465-42-8P  
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 IT 33492-89-6P 33492-91-0P 33492-93-2P  
 33492-94-3P  
 (preparation of)  
 RN 33492-89-6 USPATFULL  
 CN Pyridinium, 1-[[2-carboxy-8-oxo-7-(2-phenylacetamido)-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl]-, bromide, 2,2,2-trichloroethyl ester, S-oxide, stereoisomer (8CI) (CA INDEX NAME)



● Br<sup>-</sup>

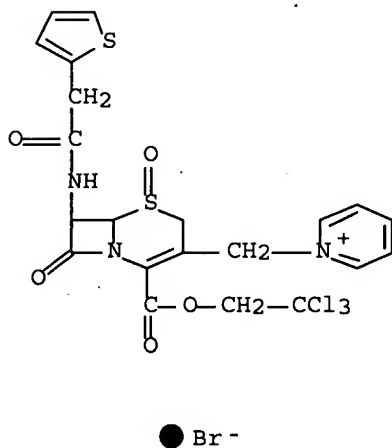
RN 33492-91-0 USPATFULL

CN Pyridinium, 1-[[2-carboxy-8-oxo-7-(2-phenylacetamido)-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl]-3-[(hydroxymethyl)carbamoyl]-, bromide, 2,2,2-trichloroethyl ester, S-oxide, stereoisomer (8CI) (CA INDEX NAME)



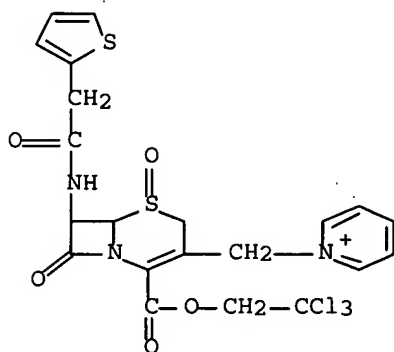
RN 33492-93-2 USPATFULL

CN Pyridinium, 1-[[2-carboxy-8-oxo-7-[2-(2-thienyl)acetamido]-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl]-, bromide, 2,2,2-trichloroethyl ester, 5-oxide, stereoisomer (8CI) (CA INDEX NAME)



RN 33492-94-3 USPATFULL

CN Pyridinium, 1-[[5-oxido-8-oxo-7-[(2-thienylacetyl)amino]-2-[(2,2,2-trichloroethoxy)carbonyl]-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl]-, chloride, [5S-(5α,6β,7α)]- (9CI) (CA INDEX NAME)



● Cl -

L28 ANSWER 10 OF 13 USPATFULL on STN

ACCESSION NUMBER: 78:47489 USPATFULL Full-text

TITLE: Process for the preparation of 3-vinyl and substituted vinyl cephalosporins

INVENTOR(S): Clark, John C., Gerrards Cross, Great Britain  
Kennedy, James, Angus, Great Britain  
Long, Alan G., Greenford, Great Britain  
Weir, Niall G., London, Great Britain

PATENT ASSIGNEE(S): Glaxo Laboratories Limited, Greenford, Great Britain  
(non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 4110534		19780829
APPLICATION INFO.:	US 1976-679073		19760421 (5)
RELATED APPLN. INFO.:	Division of Ser. No. US 1974-486633, filed on 8 Jul 1974, now Defensive Publication No. which is a continuation of Ser. No. US 1971-108136, filed on 20 Jan 1971, now abandoned		

	NUMBER	DATE
PRIORITY INFORMATION:	GB 1970-3464	19700123
	GB 1970-21907	19700123
	GB 1970-28194	19700123

DOCUMENT TYPE: Utility  
FILE SEGMENT: Granted  
PRIMARY EXAMINER: Rizzo, Nicholas S.  
LEGAL REPRESENTATIVE: Bacon & Thomas  
NUMBER OF CLAIMS: 10  
EXEMPLARY CLAIM: 1  
LINE COUNT: 3342

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention is concerned with the preparation of  $\Delta$ .sup.3 -4-carboxy cephalosporin antibiotics possessing a 3-vinyl group or substituted 3-vinyl group by means of phosphorous intermediates.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

SUMM . . . by thin layer chromatography and by ultra-violet spectroscopy (in general, the  $\lambda_{\text{sub.max}}$  shifts to higher wavelengths as the reaction produces *chromophoric* groups). Disappearance of the 3-formyl group is complete when no fraction on the chromatograms goes red or orange with 2,4-dinitrophenylhydrazine.

DETD Treatment of this material in ethanol solution with ethoxycarbonylmethylenetriphenylphosphorane (pKa 8.95) gave no *chromophore* at 388 nm corresponding to the phosphorane derived from the title compound. However, treatment with carbamoylmethylenetriphenylphosphorane (pKa 11) gave the *chromophore* at 388 nm, corresponding to the phosphorane (pKa values in 80%-aqueous ethanol determined by S. Fliszar, R. F. Hudson and. . .

DETD . . . (2 ml.) and 5% aqueous sodium bicarbonate solution (5 ml.) and the mixture stirred vigorously at room temperature until the *chromophore* of the starting material at 388 nm. had disappeared (ca. 30 minutes). The organic layer was separated and washed with. . .

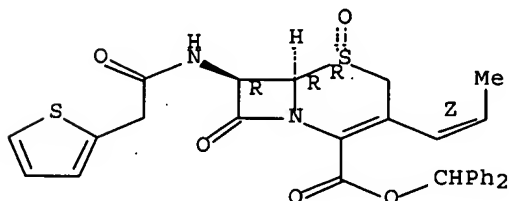
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 34712-49-7P  
 (preparation of)

IT 33747-84-1P  
 (preparation of)

RN 33747-84-1 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
 8-oxo-3-(1-propenyl)-7-[(2-thienylacetyl)amino]-, diphenylmethyl ester,  
 5-oxide, [5R-[3(Z),5 $\alpha$ ,6 $\alpha$ ,7 $\beta$ ]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



L28 ANSWER 11 OF 13 USPATFULL on STN

ACCESSION NUMBER: 78:44172 USPATFULL Full-text  
TITLE:  $\Delta$ .sup.3 -3-Vinyl or substituted vinyl-4-carboxy  
cephalosporins  
INVENTOR(S): Clark, John Colin, Gerrards Cross, England  
Kennedy, James, Angus, Scotland  
Long, Alan Gibson, Greenford, England  
Weir, Niall Galbraith, London, England  
PATENT ASSIGNEE(S): Glaxo Laboratories Limited, Greenford, England  
(non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 4107431		19780815
APPLICATION INFO.:	US 1974-486633		19740708 (5)
RELATED APPLN. INFO.:	Continuation of Ser. No. US 1971-108136, filed on 20 Jan 1971, now abandoned		

	NUMBER	DATE
PRIORITY INFORMATION:	GB 1970-3436	19700123
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	Granted	
PRIMARY EXAMINER:	Tovar, Jose	
LEGAL REPRESENTATIVE:	Bacon & Thomas	
NUMBER OF CLAIMS:	13	
EXEMPLARY CLAIM:	1	
LINE COUNT:	3289	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention is concerned with  $\Delta$ .sup.3 -4-carboxy cephalosporin antibiotics possessing a 3-vinyl or substituted 3-vinyl groups as well as with phosphorous intermediates useful in the preparation thereof.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

SUMM . . . by thin layer chromatography and by ultra-violet spectroscopy (in general, the  $\lambda_{max}$  shifts to higher wavelengths as the reaction produces *chromophoric* groups). Disappearance of the 3-formyl group is complete when no fraction on the chromatograms goes red or orange with 2,4-dinitrophenylhydrazine.

DETD Treatment of this material in ethanol solution with ethoxycarbonylmethylenetriphenylphosphorane (pKa 8.95) gave no *chromophore* at 388 nm corresponding to the phosphorane derived from the title compound. However, treatment with carbamoylmethylenetriphenylphosphorane (pKa 11) gave the *chromophore* at 388 nm, corresponding to the phosphorane (pKa values in 80%-aqueous ethanol determined by S. Fliszar, R. F. Hudson and. . .

DETD . . . (2 ml.) and 5% aqueous sodium bicarbonate solution (5 ml.) and the mixture stirred vigorously at room temperature until the *chromophore* of the starting material at 388 nm. had disappeared (ca. 30 minutes). The organic layer was separated and washed with. . .

IT 979-94-2P 30200-18-1P 33741-83-2P 33741-85-4P 33741-87-6P  
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(preparation of)

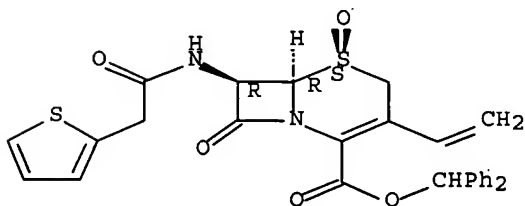
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(preparation of)

RN 69166-19-4 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
3-ethenyl-8-oxo-7-[(2-thienylacetyl)amino]-, diphenylmethyl ester,  
5-oxide, [5S-(5 $\alpha$ ,6 $\beta$ ,7 $\alpha$ )]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

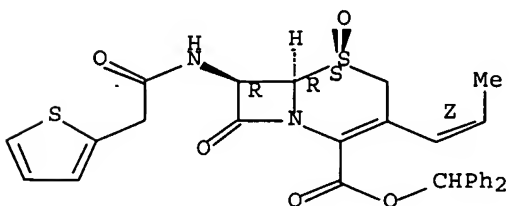


RN 69166-20-7 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
8-oxo-3-(1-propenyl)-7-[(2-thienylacetyl)amino]-, diphenylmethyl ester,  
5-oxide, [5S-[3(Z),5 $\alpha$ ,6 $\beta$ ,7 $\alpha$ ]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



L28 ANSWER 12 OF 13 USPATFULL on STN

ACCESSION NUMBER: 76:64940 USPATFULL Full-text

TITLE: 3-Vinyl-7 $\beta$ -(2,2-disubstituted acetamido)-  
cephalosporins

INVENTOR(S): Weir, Niall Galbraith, London, England

PATENT ASSIGNEE(S): Glaxo Laboratories Limited, Greenford, England  
(non-U.S. corporation)



	NUMBER	KIND	DATE
PATENT INFORMATION:	US 3994884		19761130
APPLICATION INFO.:	US 1974-440753		19740208 (5)
RELATED APPLN. INFO.:	Continuation of Ser. No. US 1971-108134, filed on 20 Jan 1971, now abandoned		

	NUMBER	DATE
PRIORITY INFORMATION:	GB 1970-28194	19700610
	GB 1971-346470	19710112
	GB 1971-2190770	19710112
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	Granted	
PRIMARY EXAMINER:	Rizzo, Nicholas S.	
LEGAL REPRESENTATIVE:	Bacon & Thomas	
NUMBER OF CLAIMS:	5	
EXEMPLARY CLAIM:	1	
LINE COUNT:	1705	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention is concerned with  $\Delta$ .sup.3 -4-carboxy cephalosporin antibiotics possessing a 3-vinyl group and having 2,2-disubstituted acetamido group at the 7-position.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

DETD Treatment of this material in ethanol solution with ethoxycarbonylmethylenetriphenylphosphorane (pKa 8.95) gave no **chromophore** at 388 nm corresponding to the phosphorane derived from the title compound. However, treatment with carbamoylmethylenetriphenylphosphorane (pKa 11) gave the **chromophore** at 388 nm, corresponding to the phosphorane (pKa values in 80%-aqueous ethanol determined by S. Fliszar, R. F. Hudson and.

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(preparation of)

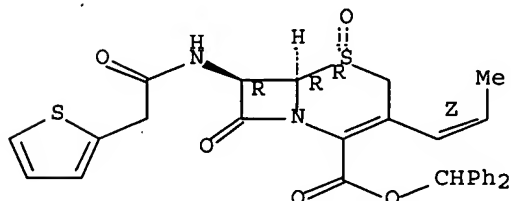
IT 33747-84-1P

(preparation of)

RN 33747-84-1 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
8-oxo-3-(1-propenyl)-7-[(2-thienylacetyl)amino]-, diphenylmethyl ester,  
5-oxide, [5R-[3(Z),5 $\alpha$ ,6 $\alpha$ ,7 $\beta$ ]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



L28 ANSWER 13 OF 13 USPATFULL on STN  
ACCESSION NUMBER: 76:2206 USPATFULL Full-text  
TITLE: 3-R-methyl-7-amino-ceph-em-4-carboxylic acid compounds  
INVENTOR(S): Peter, Heinrich, Riehen, Switzerland  
Rodriguez, Herman Robert, New York, NY, United States  
Bickel, Hans, Binningen, Switzerland  
PATENT ASSIGNEE(S): Ciba-Geigy Corporation, Ardsley, NY, United States  
(U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 3932465		19760113
APPLICATION INFO.:	US 1971-159527		19710702 (5)

	NUMBER	DATE
PRIORITY INFORMATION:	CH 1970-10305	19700708
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	Granted	
PRIMARY EXAMINER:	Rizzo, Nicholas S.	
LEGAL REPRESENTATIVE:	Kolodny, Joseph G., Maitner, John J., Groeger, Theodore O.	
NUMBER OF CLAIMS:	10	
EXEMPLARY CLAIM:	1	
LINE COUNT:	4827	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB 3-R-Methyl-7-amino-ceph-2-em-4 $\xi$ -carboxylic acid compounds, in which R is the C-residue of a C-nucleophilic compound are valuable intermediates, for example, in the manufacture of the corresponding 3-R-methyl-7-amino-ceph-3-em-4-carboxylic acid compounds with antibiotic properties.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

DETD . . . 164°-164.5° (with decomp.; uncorr.);  
[ $\alpha$ ].sub.D.sup.20 = 198°  $\pm$  1° (c = 1.007 in dioxane); thin-layer chromatogram (silica gel, plates with fluorescence indicator; detection with ultraviolet light  $\lambda$  = 254 m $\mu$  and iodine vapour): Rf = 0.72 (system:n-butanol/acetic acid/water 75:7.5:21), Rf = . . .  
DETD . . . at 174.5°-176° (with decomposition) after drying

15 hours under a high vacuum at 35°; thin-layer chromatogram (silica gel; plates with *fluorescence* indicator; detection with ultraviolet light  $\lambda = 254$  m $\mu$  and iodine vapour): Rf = 0.71 (system: n-butanol/acetic acid/water 75:7.5:21), Rf. . .

DETD . . . over anhydrous magnesium sulphate and evaporated under reduced pressure. The residue is placed onto preparative thin-layer plates (silica gel, with *fluorescence* indicator). The plates are developed during approximately 5 hours in the system n-butanol/glacial acetic acid/water (44:12:44). After drying, the main. . .

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(preparation of)

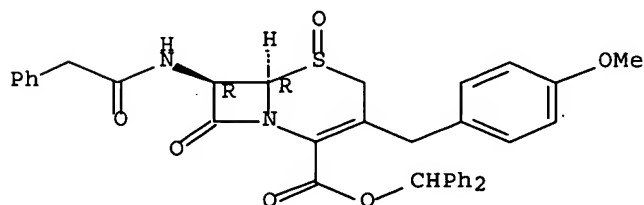
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(preparation of)

RN 36242-73-6 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
 3-[(4-methoxyphenyl)methyl]-8-oxo-7-[(phenylacetyl)amino]-,  
 diphenylmethyl ester, 5-oxide, [6R-(6 $\alpha$ ,7 $\beta$ )]- (9CI) (CA INDEX  
 NAME)

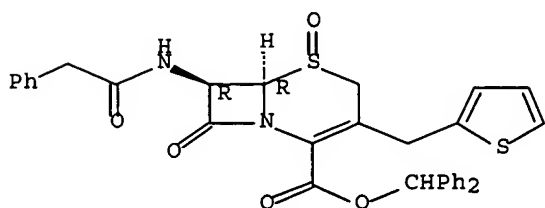
Absolute stereochemistry.



RN 36242-74-7 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
 8-oxo-7-[(phenylacetyl)amino]-3-(2-thienylmethyl)-, diphenylmethyl  
 ester, 5-oxide, [6R-(6 $\alpha$ ,7 $\beta$ )]- (9CI) (CA INDEX NAME)

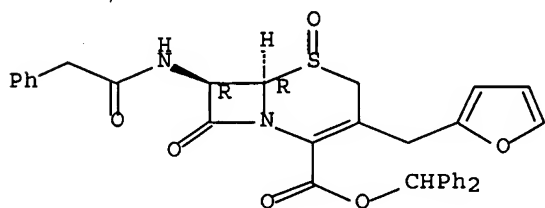
Absolute stereochemistry.



RN 36242-75-8 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
3-(2-furanylmethyl)-8-oxo-7-[(phenylacetyl)amino]-, diphenylmethyl  
ester, 5-oxide, [6R-(6 $\alpha$ ,7 $\beta$ )]- (9CI) (CA INDEX NAME)

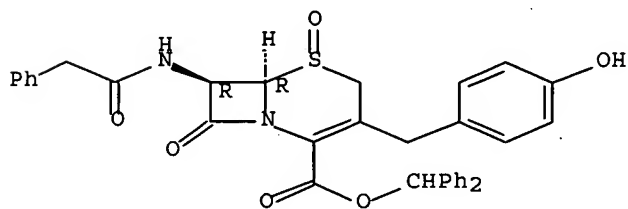
Absolute stereochemistry.



RN 36242-76-9 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
3-[(4-hydroxyphenyl)methyl]-8-oxo-7-[(phenylacetyl)amino]-,  
diphenylmethyl ester, 5-oxide, [6R-(6 $\alpha$ ,7 $\beta$ )]- (9CI) (CA INDEX  
NAME)

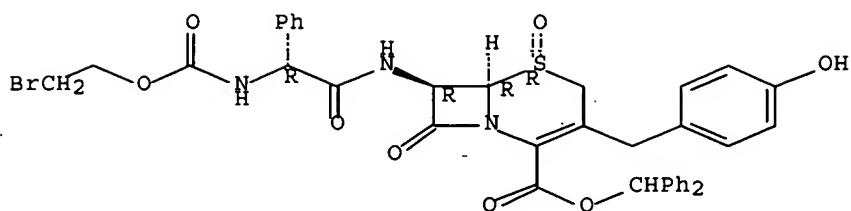
Absolute stereochemistry.



RN 36242-77-0 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
7-[[[(2-bromoethoxy)carbonyl]amino]phenylacetyl]amino]-3-[(4-  
hydroxyphenyl)methyl]-8-oxo-, diphenylmethyl ester, 5-oxide,  
[5R-[5 $\alpha$ ,6 $\alpha$ ,7 $\beta$ (R\*)]]- (9CI) (CA INDEX NAME)

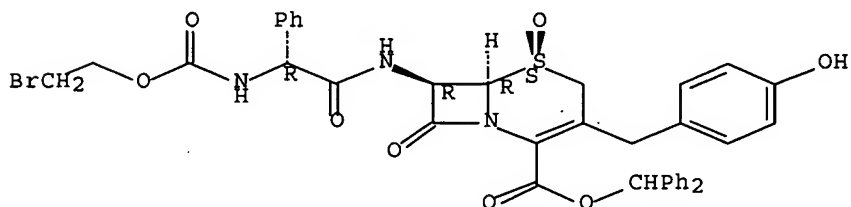
Absolute stereochemistry.



RN 36242-78-1 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
7-[[[(2-bromoethoxy)carbonyl]amino]phenylacetyl]amino]-3-[(4-  
hydroxyphenyl)methyl]-8-oxo-, diphenylmethyl ester, 5-oxide,  
[5S-[5 $\alpha$ ,6 $\beta$ ,7 $\alpha$ (S\*)]]- (9CI) (CA INDEX NAME)

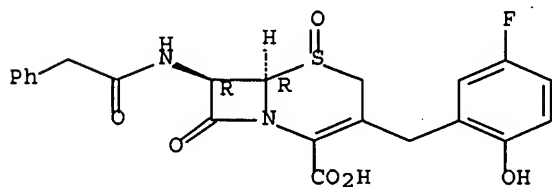
Absolute stereochemistry.



RN 36242-79-2 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
3-[(5-fluoro-2-hydroxyphenyl)methyl]-8-oxo-7-[(phenylacetyl)amino]-,  
5-oxide, [6R-(6 $\alpha$ ,7 $\beta$ )]- (9CI) (CA INDEX NAME)

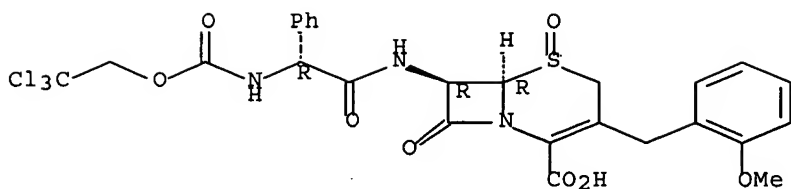
Absolute stereochemistry.



RN 36242-80-5 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
3-[(2-methoxyphenyl)methyl]-8-oxo-7-[[[(2,2,2-  
trichloroethoxy)carbonyl]amino]phenylacetyl]amino]-, 5-oxide,  
[6R-[6 $\alpha$ ,7 $\beta$ (R\*)]]- (9CI) (CA INDEX NAME)

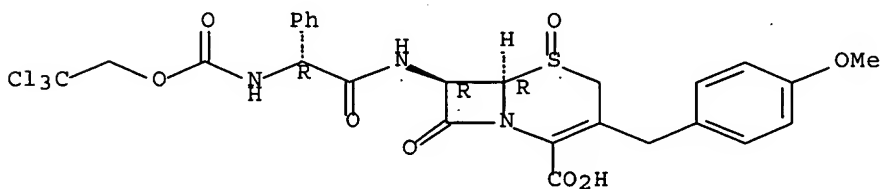
Absolute stereochemistry.



RN 36242-81-6 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
3-[(4-methoxyphenyl)methyl]-8-oxo-7-[[[(2,2,2-trichloroethoxy)carbonyl]amino]phenylacetyl]amino]-, 5-oxide,  
[6R-[6 $\alpha$ ,7 $\beta$ (R\*)]]- (9CI) (CA INDEX NAME)

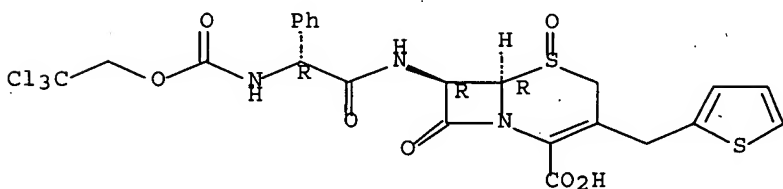
Absolute stereochemistry.



RN 36242-82-7 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
8-oxo-3-(2-thienylmethyl)-7-[[[(2,2,2-trichloroethoxy)carbonyl]amino]phenylacetyl]amino]-, 5-oxide, [6R-[6 $\alpha$ ,7 $\beta$ (R\*)]]- (9CI) (CA  
INDEX NAME)

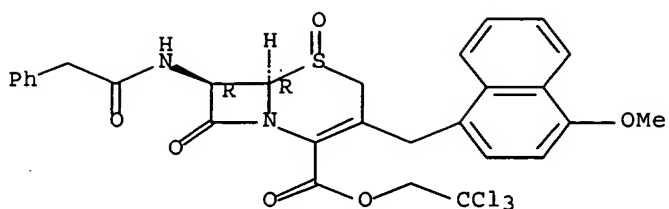
Absolute stereochemistry.



RN 36406-59-4 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
3-[(4-methoxy-1-naphthalenyl)methyl]-8-oxo-7-[(phenylacetyl)amino]-, 2,2,2-trichloroethyl ester, 5-oxide, [6R-(6 $\alpha$ ,7 $\beta$ )]- (9CI) (CA  
INDEX NAME)

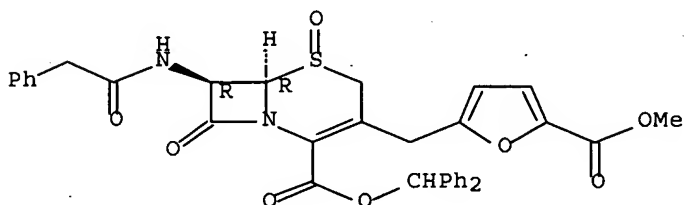
Absolute stereochemistry.



RN 36406-60-7 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
3-[[5-(methoxycarbonyl)-2-furanyl]methyl]-8-oxo-7-[(phenylacetyl)amino]-  
, diphenylmethyl ester, 5-oxide, [6R-(6 $\alpha$ ,7 $\beta$ )]- (9CI) (CA  
INDEX NAME)

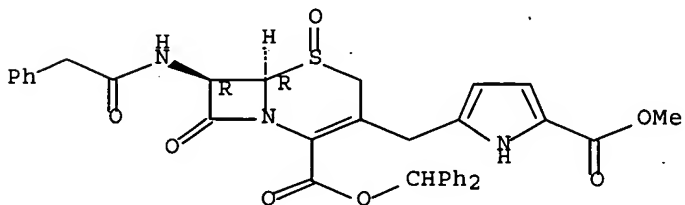
Absolute stereochemistry.



RN 36406-61-8 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
3-[[5-(methoxycarbonyl)-1H-pyrrol-2-yl]methyl]-8-oxo-7-  
[(phenylacetyl)amino]-, diphenylmethyl ester, 5-oxide,  
[6R-(6 $\alpha$ ,7 $\beta$ )]- (9CI) (CA INDEX NAME)

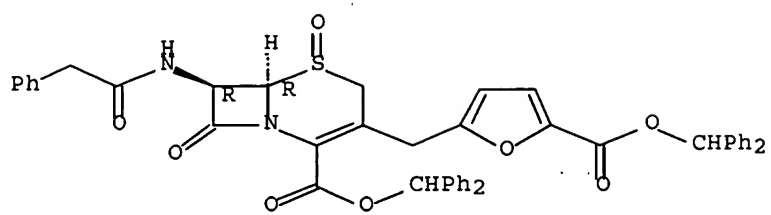
Absolute stereochemistry.



RN 36488-97-8 USPATFULL

CN 5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,  
3-[[5-[(diphenylmethoxy)carbonyl]-2-furanyl]methyl]-8-oxo-7-  
[(phenylacetyl)amino]-, diphenylmethyl ester, 5-oxide,  
[6R-(6 $\alpha$ ,7 $\beta$ )]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.





=> d his full

(FILE 'HOME' ENTERED AT 14:31:03 ON 11 DEC 2006)

FILE 'REGISTRY' ENTERED AT 14:31:07 ON 11 DEC 2006

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D SCA  
L3 178 SEA SSS FUL L1  
SAVE TEMP L3 BER486STR1L/A

FILE 'CAPLUS' ENTERED AT 14:34:05 ON 11 DEC 2006

L4 82 SEA ABB=ON PLU=ON L3  
L5 4869 SEA ABB=ON PLU=ON ?FLUOROGEN?/BI  
D KWIC 1-3  
E ?FLUORESCEN?/BI  
L6 484544 SEA ABB=ON PLU=ON ?FLUORESCEN?/BI  
L7 380423 SEA ABB=ON PLU=ON DYE?/BI  
L8 381931 SEA ABB=ON PLU=ON ?DYE?/BI  
L9 39403 SEA ABB=ON PLU=ON ?CHROMOPHOR?/BI  
L10 7 SEA ABB=ON PLU=ON L4 AND (L5 OR L6 OR L7 OR L8 OR L9)  
D SCA

FILE 'STNGUIDE' ENTERED AT 14:37:07 ON 11 DEC 2006

FILE 'CAPLUS' ENTERED AT 14:38:10 ON 11 DEC 2006

E US2002-044486/APPS  
L11 1 SEA ABB=ON PLU=ON US2002-044486/APPS  
D SCA  
L12 1 SEA ABB=ON PLU=ON L10 AND L11  
L13 11130 SEA ABB=ON PLU=ON ?FLUOROPHOR?/BI  
L14 1 SEA ABB=ON PLU=ON L4 AND L13

FILE 'USPATFULL' ENTERED AT 14:40:19 ON 11 DEC 2006

L15 36 SEA ABB=ON PLU=ON L3  
L16 6627 SEA ABB=ON PLU=ON ?FLUOROGEN?  
L17 208657 SEA ABB=ON PLU=ON ?FLUORESCEN?  
L18 267900 SEA ABB=ON PLU=ON DYE?  
L19 20051 SEA ABB=ON PLU=ON ?CHROMOPHOR?  
L20 18544 SEA ABB=ON PLU=ON ?FLUOROPHOR?  
L21 11 SEA ABB=ON PLU=ON L15 AND (L16 OR L17 OR L18 OR L19 OR L20)

FILE 'CAPLUS' ENTERED AT 14:42:08 ON 11 DEC 2006

SEL PN L10

FILE 'USPATFULL' ENTERED AT 14:42:53 ON 11 DEC 2006

L22 5 SEA ABB=ON PLU=ON (WO2002068678/PN OR WO2004090104/PN OR  
WO2005059163/PN OR WO2005071096/PN OR CA2434679/PN OR EP1385853  
/PN OR EP1616032/PN OR EP1674579/PN OR EP1704244/PN OR  
EP17111504/PN OR JP2005501806/PN OR US2003003526/PN OR US2005118  
669/PN OR US2005181469/PN OR US2005227309/PN OR US2005244907/PN  
OR WO2005024049/PN OR WO2006085978/PN)  
L23 6 SEA ABB=ON PLU=ON L21 NOT L22

FILE 'CAPLUS, USPATFULL' ENTERED AT 14:43:26 ON 11 DEC 2006

L24 13 DUP REM L10 L23 (0 DUPLICATES REMOVED)  
ANSWERS '1-7' FROM FILE CAPLUS  
ANSWERS '8-13' FROM FILE USPATFULL

FILE 'CAPLUS' ENTERED AT 14:43:45 ON 11 DEC 2006  
SEL AN L10

L25 FILE 'USPATFULL' ENTERED AT 14:43:59 ON 11 DEC 2006  
1 SEA ABB=ON PLU=ON ("137:197525"/AN OR "139:287990"/AN OR  
"141:389858"/AN OR "142:312727"/AN OR "143:189108"/AN OR  
"143:22126"/AN OR "143:93614"/AN OR "2002:676218"/AN OR  
"2003:643607"/AN OR "2004:878473"/AN OR "2005:239156"/AN OR  
"2005:474830"/AN OR "2005:571011"/AN OR "2005:697024"/AN)  
L26 0 SEA ABB=ON PLU=ON L25 AND L23

FILE 'USPATFULL' ENTERED AT 14:44:44 ON 11 DEC 2006  
D KWIC L23 1-6

FILE 'CAPLUS' ENTERED AT 14:46:28 ON 11 DEC 2006  
SEL HIT RN L10

L27 FILE 'REGISTRY' ENTERED AT 14:46:45 ON 11 DEC 2006  
18 SEA ABB=ON PLU=ON (452280-30-7/BI OR 452280-31-8/BI OR  
609812-89-7/BI OR 609812-90-0/BI OR 452280-32-9/BI OR 609812-78  
-4/BI OR 609812-82-0/BI OR 609812-85-3/BI OR 609812-91-1/BI OR  
847978-56-7/BI OR 847978-57-8/BI OR 852671-27-3/BI OR 852671-28  
-4/BI OR 852671-29-5/BI OR 852671-30-8/BI OR 852671-32-0/BI OR  
861669-96-7/BI OR 861670-03-3/BI)  
D SCA

FILE 'REGISTRY' ENTERED AT 14:49:25 ON 11 DEC 2006

FILE 'CAPLUS' ENTERED AT 14:50:55 ON 11 DEC 2006  
D STAT QUE L10  
D STAT QUE L14

FILE 'USPATFULL' ENTERED AT 14:51:22 ON 11 DEC 2006  
D STAT QUE L23

L28 FILE 'CAPLUS, USPATFULL' ENTERED AT 14:51:50 ON 11 DEC 2006  
13 DUP REM L10 L14 L23 (1 DUPLICATE REMOVED)  
ANSWERS '1-7' FROM FILE CAPLUS  
ANSWERS '8-13' FROM FILE USPATFULL  
D IBIB ABS HITIND HITSTR L28 1-7  
D IBIB ABS KWIC HITSTR L28 8-13

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 10 DEC 2006 HIGHEST RN 915124-84-4  
DICTIONARY FILE UPDATES: 10 DEC 2006 HIGHEST RN 915124-84-4

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<http://www.cas.org/ONLINE/UG/regprops.html>

FILE CAPLUS

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FILE LAST UPDATED: 10 Dec 2006 (20061210/ED)

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FILE STNGUIDE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Dec 8, 2006 (20061208/UP).

FILE USPATFULL

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 7 Dec 2006 (20061207/PD)

FILE LAST UPDATED: 7 Dec 2006 (20061207/ED)

HIGHEST GRANTED PATENT NUMBER: US7146645

HIGHEST APPLICATION PUBLICATION NUMBER: US2006277640

CA INDEXING IS CURRENT THROUGH 7 Dec 2006 (20061207/UPCA)

ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 7 Dec 2006 (20061207/PD)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2006

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2006

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# SEARCH REQUEST FORM

Requester's Full Name: MARK BERCH Examiner #: 59193 Date: 12/29/06  
Art Unit: 1624 Phone Number: 2-0663 Serial Number: 10044486  
Location (Bldg/Room#): 5C01 (Mailbox #): 5C18 Results Format Preferred (circle): PAPER DISK  
\*\*\*\*\*

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

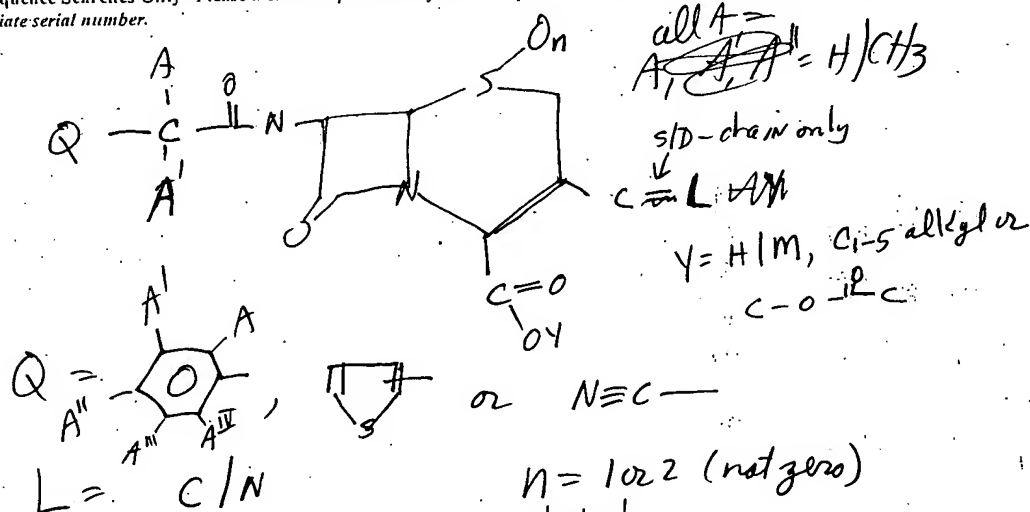
Title of Invention: \_\_\_\_\_  
Inventors (please provide full names): PULL GREEN FOLDER when two comes

Earliest Priority Date: \_\_\_\_\_ first of 2 sheets

## Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

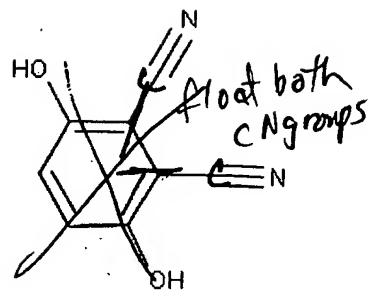
\*For Sequence Searches Only\* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.



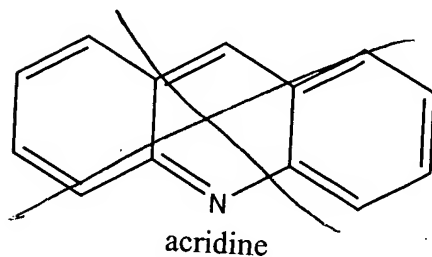
Compound must have <sup>attached</sup> linked to it one of the ~~tertiary~~ <sup>therogenic</sup> fluorescent dye, chromophore  
the groups on attached second sheet  
PY ≤ 2004

second of 2 sheets

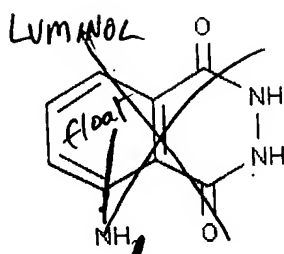
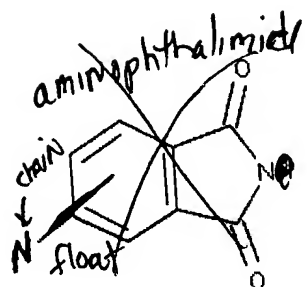
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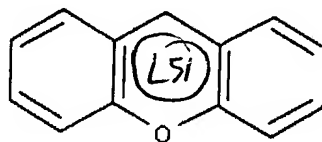
dicyanohydroquinone



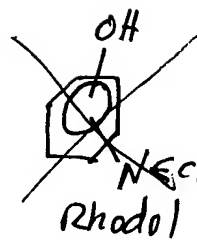
acridine



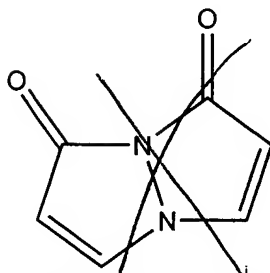
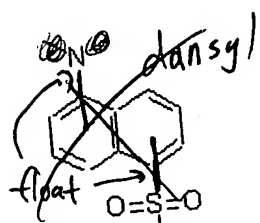
luminol



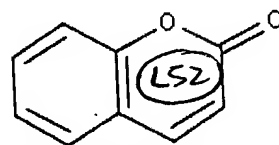
XANTHENE



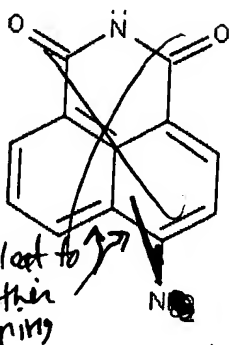
Rhodol



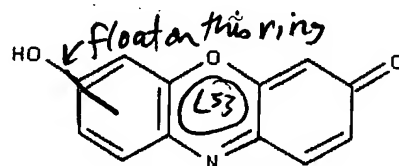
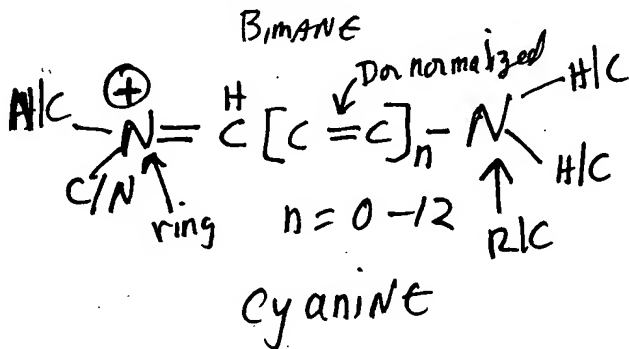
1,5-diazabicyclo[3.3.0]octa-3,6-diene-2,8-dione



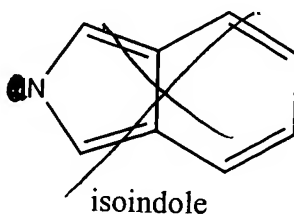
coumarin



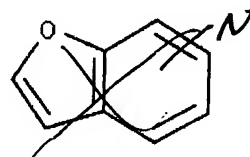
aminonaphthalimide



resorufin



isoindole



amino benzofuran

or the metal Eu or Tb